



# ievap=2: A new evaporation model. Procedure to fit pr\_evap and sc\_evap with CANTERA

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# Contents

<b>1</b>	<b>Introduction</b>	<b>3</b>
1.1	"AVBP" - The classical approach. . . . .	4
1.2	"CANTERA" - The reference. . . . .	5
1.3	"AVBPMix" - The new approach for evaporation in AVBP. . . . .	6
<b>2</b>	<b>Procedure to fit pr_evap and sc_evap with CANTERA</b>	<b>7</b>
2.1	Nasa.xml file . . . . .	7
2.2	cantevol_evap0D.choices file . . . . .	8
<b>3</b>	<b>Results</b>	<b>9</b>
	<b>Bibliography</b>	<b>14</b>

# 1 Introduction

Chauveau [3] presented recently new experimental measures for the evaporation of n-heptane droplets in the same configuration studied previously by Nomura [8]. In these experiments, a  $50\mu m$  of diameter n-heptane droplet, suspended in a quartz fiber, evaporates in a  $N_2$  quiescent atmosphere at different temperatures. The droplet diameter evolution is measured for results comparison, which showed considerable differences between the methods used by Nomura and Chauveau.

Sanjosé [9] compared the results given by AVBP with those of Chauveau and Nomura and with the results of using the complex thermodynamics of CANTERA [4] coupled with the evaporation model in AVBP. She found that the results of AVBP fitted well the results of Nomura, however, the evaporation predicted was much faster than that of Chauveau or CANTERA.

Sanjosé showed that the thermodynamical properties of the mixture have a high impact on the evaporation evolution. Afterwards, a parametric study revealed that the choice of the Pr and Sc numbers, is crucial but not sufficient to reproduce the results obtained with CANTERA. However, the implementation in AVBP of the complex laws for diffusion coefficient, thermal conductivity and dynamic viscosity used in CANTERA would be very difficult due to the use of collision potentials and CHEMKIN coefficients (cf. section 1.2). Finally, a compromise was obtained by using the Wilke's equation (eq. 12) for the viscosity with independent fittings of the viscosity as a function of temperature for each species, along with the equilibrium Prandtl and Schmidt numbers calculated with CANTERA (section 1.3). This method produced results similar to those obtained with the complex thermodynamics and transport of CANTERA (section 3). The method implies a pre-calculation with CANTERA to obtain the values of Prandtl and Schmidt numbers at equilibrium (section 2). Note that the classical approach implemented in AVBP uses the values of Prandtl and Schmidt corresponding to the chemical reduced schemes for each particular fuel, which has no physical justification regarding the evaporation process.

Finally, three different approaches for the evaporation are considered here:

- The classical approach implemented in AVBP, noted "AVBP".
- The complex thermodynamic and transport laws implemented in CANTERA, noted "CANTERA".
- The new approach, noted "AVBPMix".

in all cases, the Abramzon-Sirignano evaporation model is considered in this manuscript. However, both AVBP and the tool "CANTEVOL\_EVAP0D" presented here, may take

into account the Spalding evaporation model as well. Note also, that the tool "CAN-TEVOL-EVAP0D" calculates a 0D problem where convection effects are neglected. The equations presented here are thus simplified.

## 1.1 "AVBP" - The classical approach.

The evaporation of a liquid fuel in AVBP follows an evaporation model developed for single isolated droplet. Following the classification done by Sazhin [10], it corresponds to a model with infinite conduction in the liquid and spherical symmetry in the gas: inside the droplet, the thermal conductivity is considered infinitely fast and the temperature uniform. The gas is considered quasi-stationary, so the thermal and mass transfers in the gaseous phase depend only on the distance to the surface of the droplet.

The thermodynamic and transport properties are calculated in AVBP in a simple manner, using the reference state corresponding to the 1/3 law [6]. This law assumes that the properties in the gaseous film around the droplet follow a quasi-stationary evolution. The product  $[\rho D_F]$  can be considered as constant between the droplet surface and the infinity. AVBP evaluates this term using a constant Schmidt number for the fuel.:

$$[\rho D_F] = \frac{\mu(T_{ref})}{Sc_F}. \quad (1)$$

As it is done for the product  $[\rho D_F]$ , the thermal conductivity ( $\lambda$ ) and the heat capacity ( $C_p$ ) are evaluated at the reference state and considered constant between the droplet surface and the infinity. The evaluation of the thermal conductivity is based on a constant value for the Prandtl number of the mixture.

$$\lambda = \frac{C_p \mu(T_{ref})}{Pr} \quad (2)$$

$$C_p = \sum_{k=1}^N Y_{k,ref} C_{p,k}(T_{ref}) \quad (3)$$

The viscosity of the mixture is evaluated using a Power or Sutherland law that depends on the temperature of the reference state only.

The evolution of the evaporation of a single droplet is calculated using the Spalding (ievap=1) or the Abramzon-Sirignano model [1](ievap=11, used in this report). The mass variation is computed by integration of the fuel species conservation equation between the droplet surface and the infinity, assuming  $[\rho D_F]$  constant:

$$\frac{dm_p}{dt} = -\pi d_p Sh [\rho D_F] \ln(1 + B_M) \quad (4)$$

where  $d_p$  is the droplet diameter,  $Sh = 2$  is the Sherwood number (when the convection effects are neglected) and  $B_M = \frac{Y_{F,\zeta} - Y_{F,inf}}{1 - Y_{F,\zeta}}$  the Spalding mass number ( $\zeta$  stands for

the properties calculated at the droplet surface and  $Y_{F,\zeta}$  is calculated using the Clausius-Clapeyron law).

The heat transfert is composed by two contributions: the conductive flux ( $\Phi_g$ ) and the enthalpy flux due to phase change ( $\Lambda_g$ ):

$$\Phi_g = -\pi d_p Nu \lambda (T_{\text{inf}} - T_l) \frac{\ln(1 + B_T)}{B_T} \quad (5)$$

$$\Lambda_g = \frac{dm_p}{dt} h_{s,F}(T_l) \quad (6)$$

$Nu = 2$  is the Nusselt number (neglecting convection effects),  $B_T = (1 + B_M)^\beta$  is the thermal Spalding number ( $\beta = \frac{C_{p,F}}{C_p} \frac{ShPr}{NuSc}$ ,  $C_{p,F}$  stands for the heat capacity of gaseous fuel and  $C_p$  is the heat capacity of the mixture, both at the reference state).

## 1.2 "CANTERA" - The reference.

As reference, a formulation taking into account the complete kinetic theory will be used. It could be found, for example, on the free distribution software CANTERA [4]. The libraries on FORTRAN used to calculate the thermodynamical and transport properties on CANTERA will be coupled with a module of AVBP that calculates the evolution on time of the evaporation of a single droplet in a quiescent atmosphere using a first order iterative method. The calculation of transport and thermodynamical properties in CANTERA is based in the Chapman-Enskog kinetic theory of gases [7] and it uses the potentials of Lennard-Jones [5, 2] to calculate the intermolecular forces. The diffusion coefficient of one species into the mixture [7]:

$$D_k = \frac{1 - Y_k}{\sum_{j \neq k} X_j / D_{jk}} \quad (7)$$

where  $Y_k$  is the mass fraction of the species,  $X_j$  are the molar fractions and  $D_{jk}$  is the binary diffusion coefficient:

$$D_{jk} = \frac{3}{16} \frac{\sqrt{2\pi k_B^3 T^3 / m_{jk}}}{\pi P \sigma_{jk}^2 \Omega_{D,jk}} \quad (8)$$

here,  $m_{jk}$  is the reduced atomic mass of the pair,  $\sigma_{jk}$  the reduced collision diameter and  $\Omega_{D,jk}$  is the collision integral. The thermal conductivity of the mixture is calculated using Mathur's equation [7]:

$$\lambda = \frac{1}{2} \left( \sum_k X_k \lambda_k + \frac{1}{\sum_k X_k / \lambda_k} \right) \quad (9)$$

where the thermal conductivity of each species ( $\lambda_k$ ) depends on the geometry of the molecule. The viscosity of a single species:

$$\mu_k = \frac{5}{16} \frac{\sqrt{\pi m_k k_B T}}{\pi \sigma_k^2 \Omega_{\mu,k}} \quad (10)$$

depends on the collision diameter of the species ( $\sigma_k$ ), the mass of the molecule ( $m_k$ ), the Boltzmann's constant ( $k_B$ ) and the collision integral for the viscosity ( $\Omega_{\mu,k}$ ). The viscosity of the mixture is calculated following Wilke's equation [2]:

$$\mu = \sum_i \frac{X_i \mu_i}{\sum_j X_j \Phi_{ij}} \quad (11)$$

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{W_i}{W_j}\right)^{-1/2} \left[1 + \left(\frac{\mu_i}{\mu_j}\right)^{1/2} \left(\frac{W_j}{W_i}\right)^{1/4}\right]^2 \quad (12)$$

These properties, as well as the density of the mixture and the heat capacity are calculated at each time step at the reference state ( $T_{ref}$  and  $Y_{ref}$  calculated using the 1/3 law for the calculation of properties at the surface of the droplet [6]). Then, Prandtl and Schmidt numbers are also computed, which implies a high computational cost.

### 1.3 "AVBPMix" - The new approach for evaporation in AVBP.

A new method has been implemented in AVBP: it uses the simple thermodynamics of AVBP along with modified Prandtl and Schmidt numbers, used only for the evaporation process, calculation and the Wilke's equation (eq. 11) for the calculation of the gaseous viscosity depending on the reference temperature and composition. It can be used with the Spalding (ievap=2) or the Abramzon-Sirignano (ievap=21, used here) models.

Note that the Prandtl and Schmidt numbers used for the "AVBPMix" approach correspond to the equilibrium values obtained from a pre-calculation of the evaporation of a single isolated droplet made with CANTERA. Furthermore, they are used exclusively for the evaporation calculation and have no direct impact on the ones used for the reactive processes. Consequently, when computing two-phase evaporating and reactive cases with the new approach (ievap=2 or 21 in input\_tpf.dat file), the following files must be correctly filled:

- input\_themo.dat: the mixture viscosity law used for the gaseous phase (constant, Sutherland or Power law) must be correctly defined, the Prandtl number of the mixture must be specified too. For more information on how to fill this file can be found in [http://www.cerfacs.fr/avbp/AVBP\\_V6.X/AVBPHELP/PARAM/thermo.php](http://www.cerfacs.fr/avbp/AVBP_V6.X/AVBPHELP/PARAM/thermo.php)
- input\_premix.dat: the Schmidt numbers of all species must be those validated for the corresponding reduced chemical scheme. More information in: [http://www.cerfacs.fr/avbp/AVBP\\_V6.X/AVBPHELP/PARAM/premix.php](http://www.cerfacs.fr/avbp/AVBP_V6.X/AVBPHELP/PARAM/premix.php)
- input\_tpf.dat: line 4 must contain the Prandtl and Schmidt values issued from the pre-calculation with CANTERA. More information in: [http://www.cerfacs.fr/avbp/AVBP\\_V6.X/AVBPHELP/PARAM/tpf.php](http://www.cerfacs.fr/avbp/AVBP_V6.X/AVBPHELP/PARAM/tpf.php)

More information on the validated data for the reduced chemical schemes in AVBP can be found here: [http://www.cerfacs.fr/avbp/AVBP\\_V6.X/AVBPHELP/PARAM/chemistry/index.php](http://www.cerfacs.fr/avbp/AVBP_V6.X/AVBPHELP/PARAM/chemistry/index.php)

## 2 Procedure to fit `pr_evap` and `sc_evap` with CANTERA

All which is needed to obtain the values for `pr_evap` and `sc_evap` parameters in "input.tpf.dat" file for `ievap=2, 21` is provided by the tool `CANTEVOL_EVAP0D`.

`CANTEVOL_EVAP0D` tool calculates the 0D evaporation of a single droplet in a quasi-steady atmosphere with AVBP `ievap=1, 11, 2` and `21` models and AVBP with CANTERA thermodynamics and transport calculation for Spalding and AS evaporation models.

This tool uses a `.choices` file (`cantevol_evap0D.choices`) and a `.xml` file with the CHEMKIN coefficients for CANTERA (`Nasa_coeff.xml`).

### 2.1 Nasa.xml file

The file containing the CHEMKIN coefficients for CANTERA calculation must be named "Nasa\_coeff.xml"

The phase defined in it must have 3 dimensions and be called "gas".

All elements of all species used in the computation and the species themselves must be contained in the definition of the Nasa phase and their NASA thermo coefficients and transport parameters must be present in the file.

The file provided with the tool contains the following species: *H*, *O*, *N<sub>2</sub>*, *O<sub>2</sub>*, *H<sub>2</sub>*, *OH*, *CO*, *CO<sub>2</sub>*, *H<sub>2</sub>O*, *CH<sub>4</sub>*, *C<sub>3</sub>H<sub>8</sub>*, *C<sub>7</sub>H<sub>16</sub>*, *C<sub>8</sub>H<sub>18</sub>*, *KERO*, *KERO\_LUCHE*, *JP10*, *C<sub>10</sub>H<sub>22</sub>*, *C<sub>3</sub>H<sub>8</sub>O* and *C<sub>2</sub>H<sub>5</sub>OH*. More species can be added, provided the NASA coefficients and geometric parameters for transport properties calculation are known.

## 2.2 cantevol\_evap0D.choices file

```
'./input_premix.dat'      ! premix file
'./input_thermo.dat'     ! thermo file
'./input_species.dat'    ! species file
'./input_species_tpf.dat' ! species tpf file
'./input_tpf.dat'        ! tpf file
0                          ! iwrite, format of sol files(=1 ASCII,=2 IGOR,0=both)
1                          ! (0: no third law, 1: third law)
imodel                    ! model (do not change this line!)
5.7893E-04                ! Time step
100000                    ! nitemax
101325.0d0                ! Initial gas Pressure
0.7670d0                  ! Initial Y\1 mass fraction
0.233d0                   ! Initial Y\2 massfraction
0.0d0                     ! Initial Y\3 mass fraction
50.d-4                    ! Initial droplet diameter
688.72                    ! Droplet density (stays constant during calculation)
300.00d0                  ! Initial liquid temperature
1                          ! Number of cases

Tg   Sc_Y1   Sc_Y2   Sc_Y3   Pr
...   ...   ...   ...   ...
```

1. The first 5 lines specify the paths for *input\_premix.dat*, *input\_thermo.dat*, *input\_species.dat*, *input\_species\_tpf.dat* and *input\_tpf.dat* files.
2. "iwrite" (on line 6) specifies the format for the solution files: 1 for ASCII files, 2 for IGOR format and 0 to obtain both. 3 ASCII files corresponding to avbp\_mmm, avbp\_mmm\_tpf and avbp.dat files will be created for each evaporation model (Spalding (ievap=1/2) or AS (ievap=11/21)), each thermodynamics model (AVBP (imodel=1/3) and CANTERA (imodel=2)) and each case (specified by the user). With the following names:

- avbp\_mmm.imodel#\_ievap#\_case#
- avbp\_mmm\_tpf.imodel#\_ievap#\_case#
- avbp\_dat.imodel#\_ievap#\_case#

One IGOR file with the main variables for postprocessing is created if iwrite=2 or 0 is chosen, for each evaporation model, each thermodynamics model and each case:

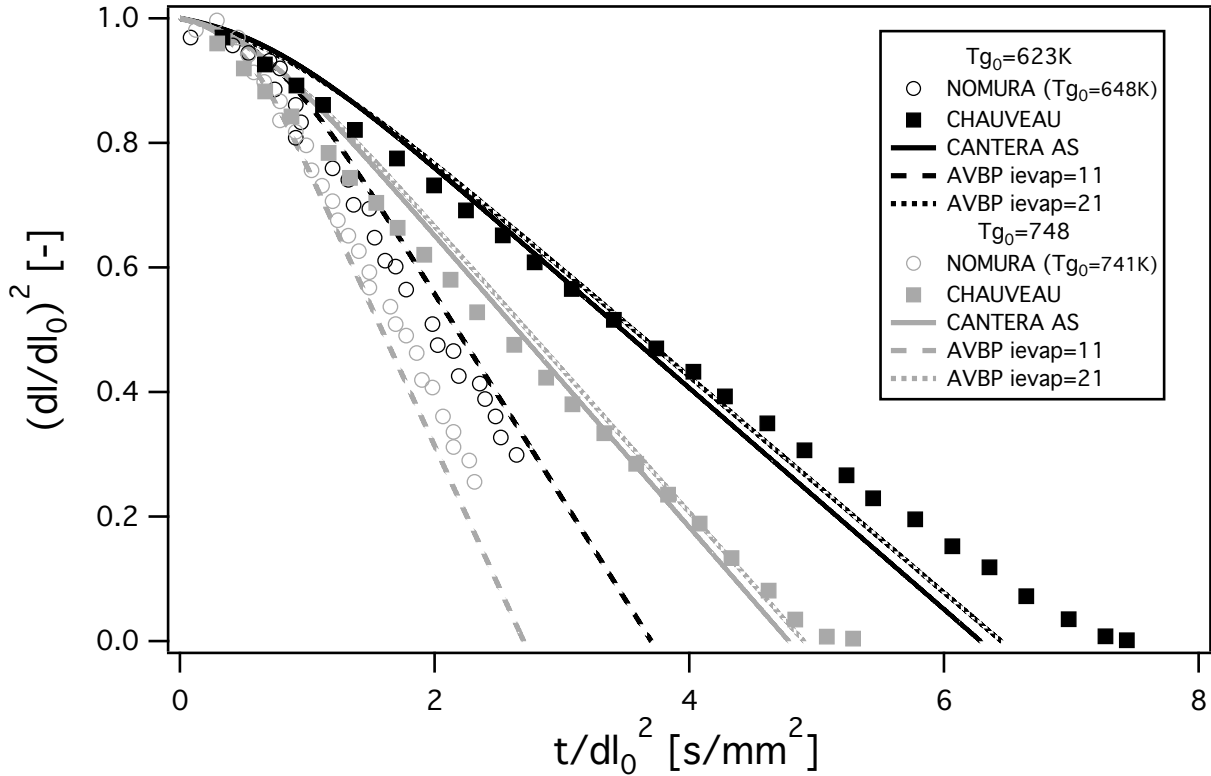
- avbp\_IGOR.imodel#\_ievap#\_case#

3. Line 7 allows to choose between using or not the  $1/3-2/3$  law for the calculation of the properties in the gaseous film around the droplet.
4. Line 8 must contain the word "imodel" only.
5. Line 9 specify the time-step for the calculation.
6. Line 10 includes the maximum number of iterations to perform (in case of saturation avoid the calculation to run indefinitely). Special attention should be given to "nitemax" and "Time step" values. "nitemax" should be large enough so as to allow the completion of the evaporation process. "Time step" must be small enough to avoid calculation instabilities.
7. Line 11 gives the initial gaseous pressure.
8. This example is given for a calculation with 3 species. From line 12 on, the user must include one line for each species in the calculation giving the initial mass fraction of the species. The order of the species must be the same as in input\_premix.dat file.
9. Line 12+nspec (15 in this example) contains the initial droplet diameter (being nspec the total number of species in the calculation).
10. Line 13+nspec (16 here) contains the droplet density (stays constant during calculation).
11. Line 14+nspec (17 in this example) specifies the initial droplet temperature.
12. In line 15+nspec (18 here), the number of different cases to compute must be specified (up to 99 cases). Each case allows different initial gaseous temperatures or Schmidt and Prandtl numbers for the "AVBP" approach. The following line must be blank.
13. The file must end with one line for each case to compute, including: Tg (Initial gaseous temperature), Schmidt number for each species and mixture Prandtl number.

### 3 Results

Figure 1 shows the evolution of the adimensional droplet diameter calculated with CANTERA and both methods implemented in AVBP, as well as the experimental results of Nomura and Chauveau, for two different initial gaseous temperatures. The results of AVBP with the classical method fit the results of Nomura, however les results of Chauveau show a much slower evaporation process. The simulations with CANTERA match the slope of the curves obtained by Chauveau at the beginning of the evaporation process, however they differ at the end. Prandtl and Schmidt values for  $ievap=21$  were fitted with

the case a 623K. The new method implemented in AVBP show results close to those of CANTERA for both temperatures.



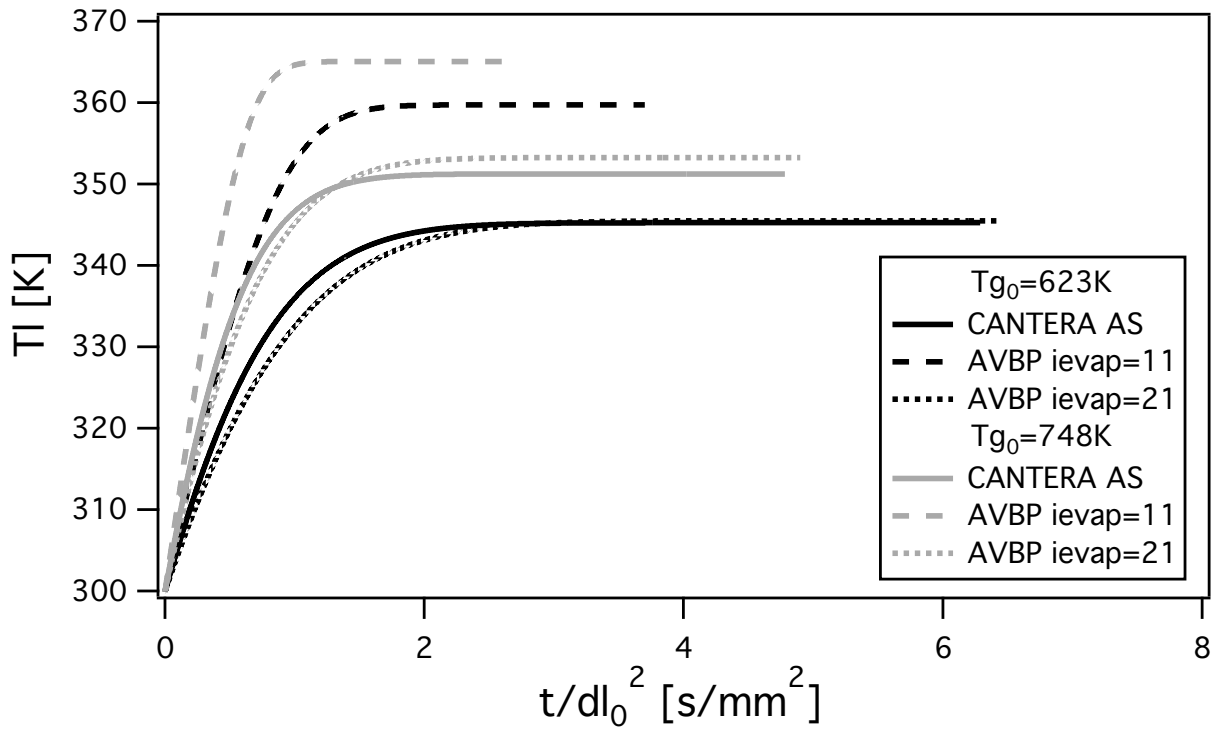
**Figure 1:** Comparison of n-heptane droplet vaporisation at 623K and 748K.

Figure 2 shows the evolution in time of the computed droplet temperature for two different initial ambient temperatures. The results of  $ie vap=11$  shows evolution and equilibrium temperatures very different of those of CANTERA.  $ie vap=21$  does not produce the same evolution of the droplet temperature. However, the equilibrium temperature is much closer to CANTERA than the one calculated with the  $ie vap=11$ .

Figure 3 shows the evolution of the gaseous properties during the evaporation process for the cases at 623K and 748K. In both cases,  $ie vap=21$  produce results very similar to those of CANTERA;  $ie vap=11$  gives very different results.

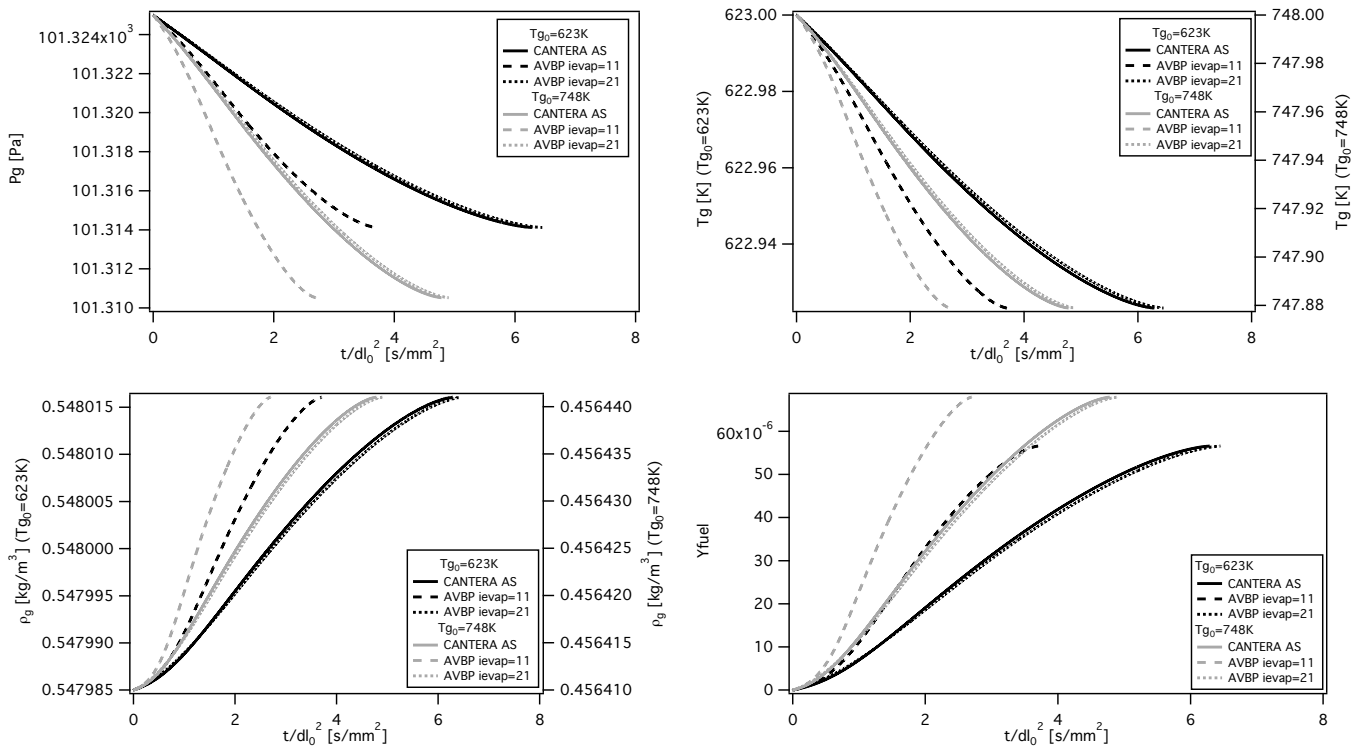
Figure 4 shows the mass and heat source terms during the evaporation. Although it is not perfect,  $ie vap=21$  produces very good results compared to  $ie vap=11$ . It reproduces the evolution of the source terms, although the maximum values are not captured.

Figure 5 shows the evolution of the thermodynamical properties during the evaporation process: the thermal conductivity is very different between CANTERA and  $ie vap=21$  and  $ie vap=11$ ; on the other hand, the diffusivity does not vary much. This is due to the large

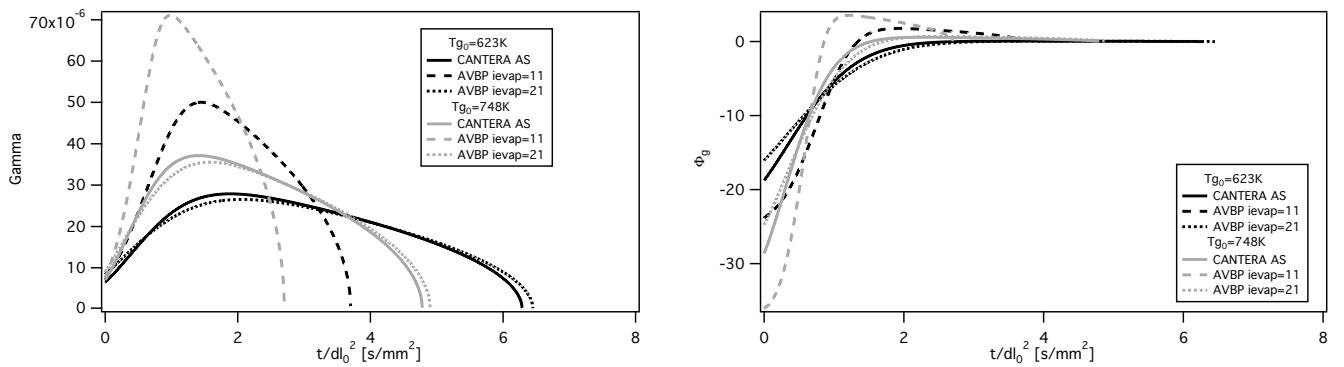


**Figure 2:** Temporal evolution of the droplet temperature for two different ambient temperatures: 623K and 748K

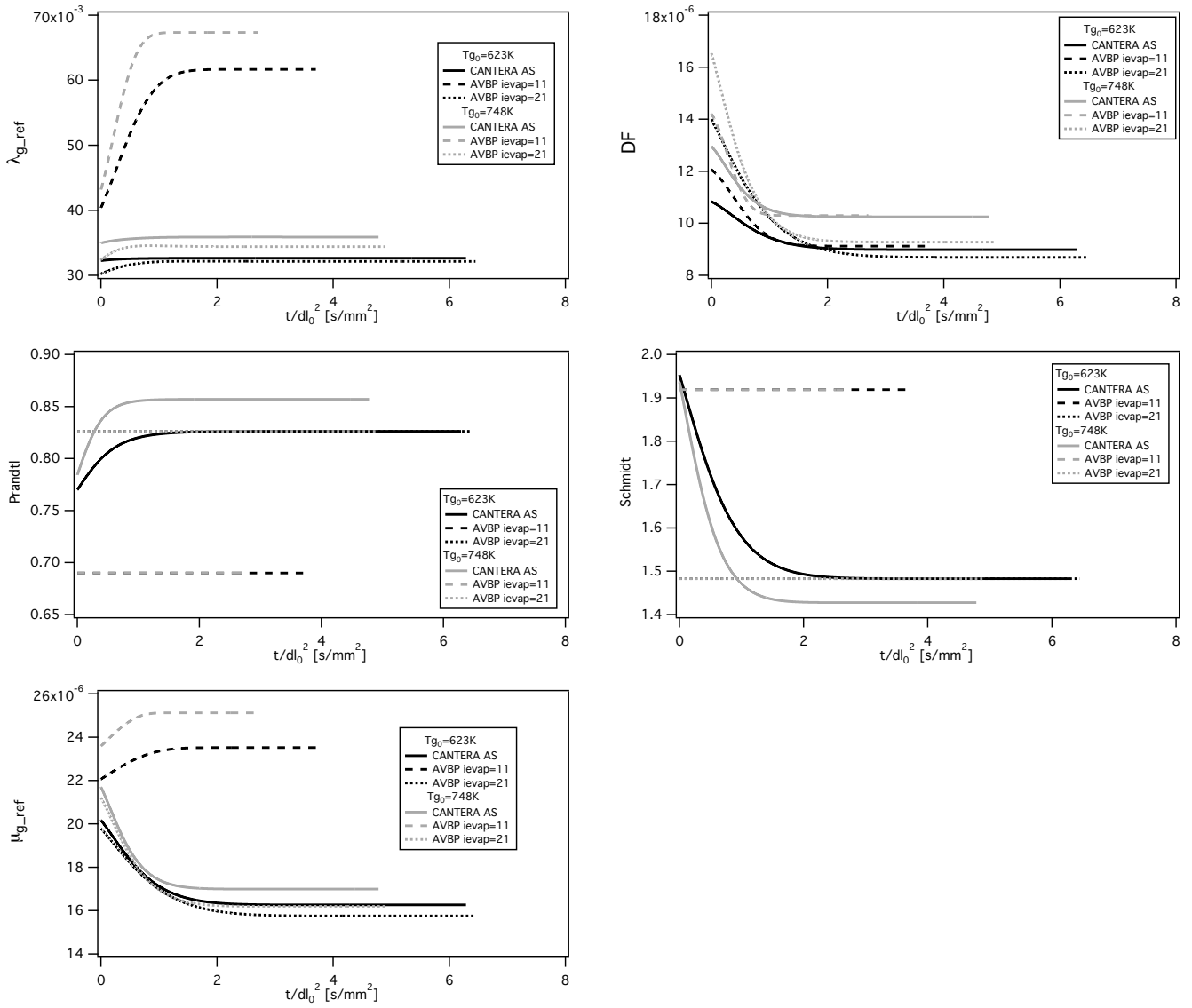
difference on the Prandtl and Schmidt numbers between CANTERA (and  $ievap=21$ ) and  $ievap=11$ , and the viscosity.



**Figure 3:** Temporal evolution of the gaseous pressure, temperature and density and fuel vapour mass fraction for two different ambient temperatures: 623K and 748K



**Figure 4:** Temporal evolution of the mass and thermal source terms.



**Figure 5:** Evolution of the thermodynamical properties.

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