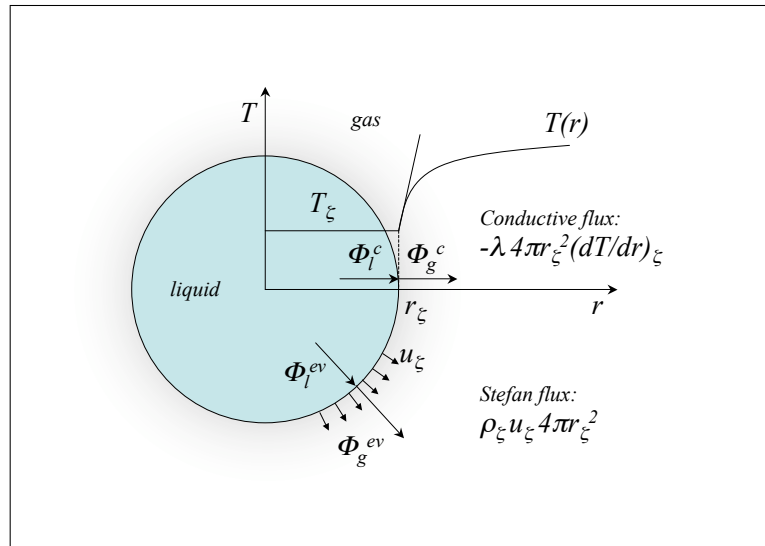




CORRECTION OF THE REFERENCE TEMPERATURE FOR THE LIQUID ENTHALPY CALCULATION IN AVBP

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Contents

1	Introduction	3
1.1	Evaporation model	3
1.2	Reference temperatures	3
2	Correction in the 'old' version of AVBP	3
3	Modification of the reference temperature for the liquid enthalpy	4
4	Comparison of the evaporation equations for Spalding model	5
4.1	Eulerian version	5
4.2	Lagrangian version	7
5	How to build a Latent heat of vaporisation table	7
6	Comparison of results	9
6.1	Comparison of results: EE - EL (AVBP_V6.1.4 tagged)	10
6.2	Comparison of results: EE AVBP_V6.1.4 tagged - EE AVBP_V6.1.4 modified.	11
6.3	Comparison of results: EL AVBP_V6.1.4 tagged - EL AVBP_V6.1.4 modified	12
	Bibliography	13

1 Introduction

There are two versions of the code AVBP: in the first one the droplets or particles are followed individually in a Lagrangian reference frame [[5],[4]], alternatively, the other version uses an Eulerian approach [[2],[3]] where the particles are described as a continuum and the phases are coupled through interphase exchange terms.

The transported variables in both versions of the code are the same, except the thermal variable: while the Lagrangian version (EL) transports the temperature of each particle, in the Eulerian version (EE) it is the enthalpy that is transported. This fact have an effect on the equations calculated for the computation of the evaporation process of a droplet.

1.1 Evaporation model

The evaporation models used in AVBP are described in the Handbook [CITE]. The first one is an equilibrium law based on the Spalding mass-transfer model. The second is the so called Abramzon-Sirignano model [[1]].

1.2 Reference temperatures

In the equations used in AVBP, a correction term arise from the difference of reference temperatures between the gaseous and the liquid enthalpies: while the gaseous enthalpy table is referred to a reference temperature of 0K, the liquid enthalpy is calculated from constant latent heat of vaporisation and constant heat capacity at constant pressure for the liquid fuel, both calculated at a reference temperature that depends on the fuel. These data are given in the 'input_species_tpf.dat' file, for all fuels.

It is possible, however, to change the reference temperature for the liquid enthalpy using a table of latent heat of vaporisation for the range of temperatures between 0K and the critical temperature particular to each fuel.

This report shows the modifications in AVBP needed to remove the correction, along with a comparison of the results in a test case obtained from the Lagrangian QPF Evap1D.

2 Correction in the 'old' version of AVBP

The difference in the reference temperature between the gaseous and liquid enthalpies made a correction arise in the code. In the equation for the variation of the droplet temperature, the latent heat of vaporisation of the liquid fuel at the droplet temperature appears (the subscript ζ represents the droplet surface):

$$\frac{dT_p}{dt} = \frac{1}{m_p C_{p,l}} (-\Phi_g^c + \dot{m}_p L_v(T_\zeta)) \quad (1)$$

Equation 1 is exact if the enthalpies of the gaseous fuel $h_{s,F}$ and the liquid $h_{s,p}$ that are used to calculate $L_v(T_\zeta) = h_{s,F}(T_\zeta) - h_{s,p}(T_\zeta)$ are referred to the same reference temperature. In AVBP_V6.1.4 this is not the case, for this reason, equation 1 must be recast as:

$$\frac{dT_p}{dt} = \frac{1}{m_p C_{p,l}} (-\Phi_g^c + \dot{m}_p [h_{s,F}(T_\zeta) - h_{s,p}(T_\zeta) - h_{s,corr}]) \quad (2)$$

where the correction enthalpy $h_{s,corr}$ accounts for the change in reference temperature between gas and liquid. $h_{s,corr}$ is obtained by expressing the values of $L_v(T_{l,ref})$:

$$L_v(T_{l,ref}) = h_{s,F}(T_{l,ref}) - h_{s,corr} - \underbrace{h_{s,p}(T_{l,ref})}_0 \quad (3)$$

$$h_{s,corr} = h_{s,F}(T_{l,ref}) - L_v(T_{l,ref}) \quad (4)$$

$h_{s,F}(T_{l,ref})$ can be evaluated using the thermodynamic tables of AVBP, $L_v(T_{l,ref})$ is given in the 'input_species_tpf.dat' file.

3 Modification of the reference temperature for the liquid enthalpy

To remove the correction due to the different reference temperatures for gaseous and liquid enthalpies, C. Habchi proposed to include a thermodynamic table of latent heat of vaporisation in AVBP from which the tables of liquid enthalpy and liquid heat capacity at constant pressure can be calculated.

In AVBP there exist a thermodynamic table of gaseous enthalpy referenced to 0K. This can be used along with the table of latent heat of vaporisation to calculate the liquid enthalpy at every temperature referenced to 0K:

$$h_{s,p}(T) = h_{s,F}(T) - L_v(T) \quad (5)$$

And from the table of liquid enthalpy, the liquid heat capacity can be easily calculated:

$$C_{p,l}(T) = \frac{h_{s,p}(T + dT) - h_{s,p}(T)}{dT} \quad (6)$$

The liquid enthalpy may be obtained from this table of $C_{p,l}$ as follows:

$$h_l(T) = C_{p,l}(T) \cdot T + h_l(0) \quad (7)$$

Using the values of these tables instead of constant latent heat of vaporisation and liquid heat capacity, the correction can be removed.

The new version includes also a modification in the calculation of the saturation pressure: in AVBP_V6.1.4 tagged, the pressure at the surface of the droplet is calculated with the Clasius-Clapeyron law, eq. (8), where T_{cc} and P_{cc} correspond to an arbitrary reference point on the saturation curve (equal to $T_{l,ref}$) and R is the universal gas constant.

$$P_{F,\zeta} = P_{cc} \left(\frac{W_F L_v(T_{l,ref})}{R} \left(\frac{1}{T_{cc}} - \frac{1}{T_\zeta} \right) \right) \quad (8)$$

In the new version a table of saturation pressure as a function of the temperature is given or each fuel.

4 Comparison of the evaporation equations for Spalding model

In this section the equations for the evaporation for the Spalding model in AVBP_V6.1.4 tagged and the modified version are compared.

The same exercise can be easily done for the Abramzon-Sirignano evaporation model.

4.1 Eulerian version

In the Eulerian version of AVBP, the liquid enthalpy is transported. The following table compares the equations for the Spalding evaporation model for the case where the reference for the liquid enthalpy is taken at a temperature given in the 'input_species.tpf.dat' file for each fuel (AVBP_V6.1.4) and a modified version where the reference is taken same as for the gaseous enthalpy: 0K.

Variable	Reference temperature = $T_{l,ref}$	Reference temperature = 0K
L_v $h_l(T)$ $C_{p,l}$ $T_{l,ref}$ T_l	$L_v(T_{l,ref})$, input, constant transported @ reference $T_{l,ref}$ constant, $C_{p,l}(T_{l,ref})$, input depends on fuel, input $T_l = \frac{h_l(T)}{C_{p,l}(T_{l,ref})} + T_{l,ref}$	$L_v(T)$ from input table $H_{lat}(T)$ transported @ reference 0K $C_{p,l}(T)$ table built from $h_{liq}(T)$ table not applicable dichotomy on $h_{liq}(T)$ table
T_{ref}	third law : $T_{ref} = \frac{2}{3}T_l + \frac{1}{3}T_g$	
$h_{s,corr}$ $L_{v,corr}$ P_ζ	$h_{s,corr} = h_{s,F}(T_{l,ref}) - L_v(T_{l,ref})$ $L_{v,corr}(T_l) = h_{s,F}(T_l) - h_l(T_l) - h_{s,corr}$ Clasius-Clapeyron law	not applicable not applicable from input table $p_{sat}(T)$
Saturated conditions : $P_\zeta < P_g$		
B_M β B_T Γ Φ_g Π_g	$B_M = (Y_\zeta - Y_{F,g})/(1 - Y_\zeta)$ $\beta = Sh \cdot Pr / Nu \cdot Sc_F$ $B_T = (1 + B_M)^\beta - 1$ $\Gamma = n_l \pi d_l [\rho D_F] \ln(1 + B_M)$ $\Phi_g = n_l \pi d_l Nu \lambda (T_\zeta - T_g)^{\frac{\ln(1+B_T)}{B_T}}$ $\Pi_g = \Phi_g + \Gamma \cdot h_{s,F}(T_l)$	
Π_l	$\Pi_l = -\Pi_g + \Gamma \cdot h_{s,corr}$	$\Pi_l = -\Pi_g$
Φ_l	$\Phi_l = -\Phi_g - \Gamma \cdot L_{v,corr}(T_l)$	$\Phi_l = -\Phi_g - \Gamma \cdot L_v(T_L)$
Boiling and condensation point : $P_\zeta \geq P_g$		
B_M	B_M not defined at surface	
B_T	$B_T = C_{P,F}(T_{ref}) \cdot (T_g - T_l) / L_{v,cor}(T_l)$	$B_T = C_{P,F}(T_{ref}) \cdot (T_g - T_l) / L_v(T_l)$
Φ_g	$\Phi_g = n_l \pi d_l Nu \lambda (T_\zeta - T_g)^{\frac{\ln(1+B_T)}{B_T}}$	
Γ	$\Gamma = -\Phi_g / L_{v,corr}(T_l)$	$\Gamma = -\Phi_g / L_v(T_l)$
Π_l	$\Pi_l = -\Gamma \cdot h_l(T_l)$	$\Pi_l = -\Gamma \cdot h_l(T_l)$
Π_g Φ_l	$\Pi_g = \Phi_g + \Gamma \cdot h_{s,F}(T_l)$ $\Phi_l = 0$	

Table 1: Set of equations for the evaporation in the EE version

4.2 Lagrangian version

In the Lagrangian version of the code, the droplet temperature is transported, thus the variation of droplet temperature in a time step is calculated in the evaporation subroutine along with the variation in the mass of the particle. As it has been done for the Eulerian version, table 2 compares the equations for the evaporation for two values of the reference temperature for the liquid enthalpy: $T_{l,ref}$ and 0K.

5 How to build a Latent heat of vaporisation table

Nowadays in AVBP we dispose of latent heat of vaporisation tables for the most usual fuels used; this data has been provided by Institut Francais du Petrole (IFP). However, if a calculation with a new fuel has to be done, and there does not exist the corresponding tables, it is possible to build the tables of latent heat of vaporisation and saturation pressure needed as input for the code.

In order to do this some data is necessary: shall we suppose in here that the values of the latent heat of vaporisation ($L_{evap} = L_v(T_{l,ref})$) and the liquid heat capacity at the reference temperature ($C_{p,l}$), the critical temperature, as well as the values of pressure and temperature at one point of the saturation curve (T_{cc} and p_{cc}) are known. From this data, it is easy to build a saturation pressure table (using Clasius-Clapeyron law, eq. (8)) and a latent heat of vaporisation table using eq. (9).

$$L_v(T) = L_v(T_{l,ref}) + \int_{T_{l,ref}}^T (C_{p,g} - C_{p,l})dT \quad (9)$$

$$= L_v(T_{l,ref}) + h_{s,g}(T) - h_{s,g}(T_{l,ref}) - C_{p,l}(T - T_{l,ref}) \quad (10)$$

The saturation pressure and latent heat of vaporisation tables should be calculated from 0K to the critical temperature of the fuel every 10 K, and inserted in the 'input_species_tpf.dat' file.

Variable	Reference temperature = $T_{l,ref}$	Reference temperature = 0K
L_v $h_p(T)$ $C_{p,l}$ $T_{l,ref}$ T_p	$L_v(T_{l,ref})$, input, constant $h_p(T) = (T_p - T_{l,ref}) \cdot C_{p,l}$ constant, $C_{p,l}(T_{l,ref})$, input depends on fuel, input transported	$L_v(T)$ from input table $H_{lat}(T)$ from table $h_{liq}(T)$ $C_{p,l}(T)$ table built from $h_{liq}(T)$ table not applicable transported
T_{ref}	third law : $T_{ref} = \frac{2}{3}T_p + \frac{1}{3}T_g$	
$h_{Fg,ref}$ P_ζ	$h_{Fg,ref} = h_{s,F}(T_{l,ref})$ Clasius-Clapeyron law	not applicable from input table $p_{sat}(T)$
Saturated conditions : $P_\zeta < P_g$		
B_M β B_T $dmpdt$ Q_p Φ_g Π_g	$B_M = (Y_\zeta - Y_{F,g})/(1 - Y_\zeta)$ $\beta = Sh \cdot Pr / Nu \cdot Sc_F$ $B_T = (1 + B_M)^\beta - 1$ $dmpdt = -\pi 2r_p [\rho D_F] \ln(1 + B_M)$ $Q_p = \pi 2r_p Nu \lambda (T_g - T_p) \frac{\ln(1+B_T)}{B_T}$ $\Phi_g = -Q_p$ $\Pi_g = \Phi_g - dmpdt \cdot h_{s,F}(T_p)$	
Π_l	$\Pi_l = -\Pi_g - (h_{Fg,ref} - L_v(T_{l,ref})) \cdot dmpdt$	$\Pi_l = -\Pi_g$
dT_{pdt}	$dT_{pdt} = \frac{\frac{\Pi_l}{C_{p,l}} - (T_p - T_{l,ref}) \cdot dmpdt}{m_p}$	$dT_{pdt} = \frac{[\Pi_l + dmpdt \cdot h_p(T_p)]}{C_{p,l}(T_p) \cdot m_p}$
Boiling and condensation point : $P_\zeta \geq P_g$		
B_M	B_M not defined at surface	
B_T	$B_T = \frac{C_{P,F}(T_{ref}) \cdot (T_g - T_p)}{[h_{Fg}(T_p) - (h_{Fg,ref} - L_v(T_{l,ref})) - h_p(T_p)]}$	$B_T = C_{P,F}(T_{ref}) \cdot (T_g - T_p) / L_v(T_p)$
Q_p Φ_g	$Q_p = \pi 2r_p Nu \lambda (T_f - T_p) \frac{\ln(1+B_T)}{B_T}$ $\Phi_g = -Q_p$	
$dmpdt$ Π_l	$dmpdt = \frac{-Q_p}{[h_{Fg}(T_p) - (h_{Fg,ref} - L_v(T_{l,ref})) - h_p(T_p)]}$ $\Pi_l = dmpdt \cdot h_p(T_p)$	$dmpdt = -Q_p / L_v(T_p)$ $\Pi_l = dmpdt \cdot h_p(T_p)$
Π_g dT_{pdt}	$\Pi_g = -dmpdt \cdot h_{s,F}(T_p) + \Phi_g$ <i>zero</i>	

Table 2: Set of equations for evaporation in the EL version

6 Comparison of results

The Low Mass Loading case of the QPF Evap1D of AVBP_V5.6_EL has been performed, in an Eulerian and a Lagrangian versions, with AVBP_V6.1.4 tagged and AVBP_V6.1.4 modified where all the changes needed for the use of the saturation and latent heat of vaporisation tables have been introduced.

In the following sections the results on the gaseous source terms of evaporation are shown. Section 6.1 shows a comparison of the Eulerian and Lagrangian versions performed with AVBP_V6.1.4 tagged. Section 6.2 shows the comparison between two Eulerian calculations: one with AVBP_V6.1.4 tagged and the other with the modified version. Section 6.3 shows a comparison between two Lagrangian calculations, performed with the two versions of the code.

The graphs shown in figures 1, 2 and 3 are produced using the script 'av2igor' that uses the tool 'avbp21d'. All AVBP tools have been modified accordingly to the changes done in the SOURCES. The values of Γ_g and Π_g are stocked in the solution file, while Φ_g and Φ_l are reconstructed inside the tool as follows:

Variable	AVBP_V6.1.4 tagged	AVBP_V6.1.4 modified
Φ_g	$\Phi_g = \Pi_g - \Gamma \cdot h_{Fg}(T_l)$	
Φ_l	$\Phi_l = -\Pi_g + \Gamma \cdot (C_{p,l}(T_{l,ref})(T_l - T_{l,ref}) + h_{l,ref})$	$\Phi_l = -\Pi_g + \Gamma \cdot h_l(T_l)$

where $h_{l,ref} = h_{Fg}(T_{l,ref}) - L_v(T_{l,ref})$.

6.1 Comparison of results: EE - EL (AVBP_V6.1.4 tagged)

Figure 1 shows no difference between the Eulerian and Lagrangian computations in the tagged version of AVBP_V6.1.4.

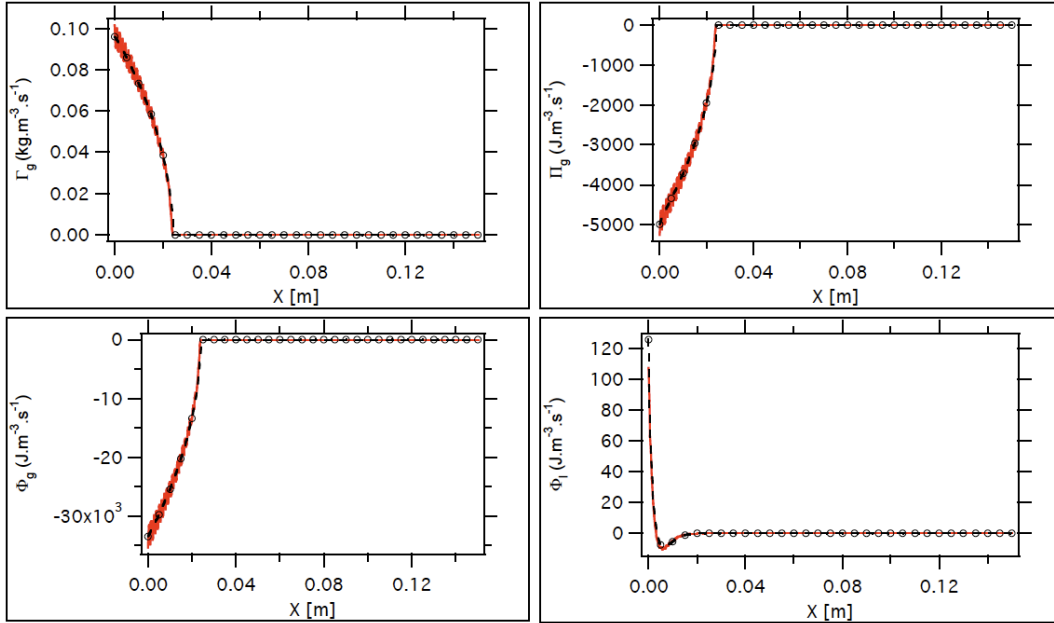


Figure 1: Comparison between EE (-o-) and EL (—) (AVBP_V6.1.4 tagged).

6.2 Comparison of results: EE AVBP_V6.1.4 tagged - EE AVBP_V6.1.4 modified.

The modifications done in AVBP in order to change the reference temperature for the liquid enthalpy produce only minor differences in the calculation, as can be seen in figure 2.

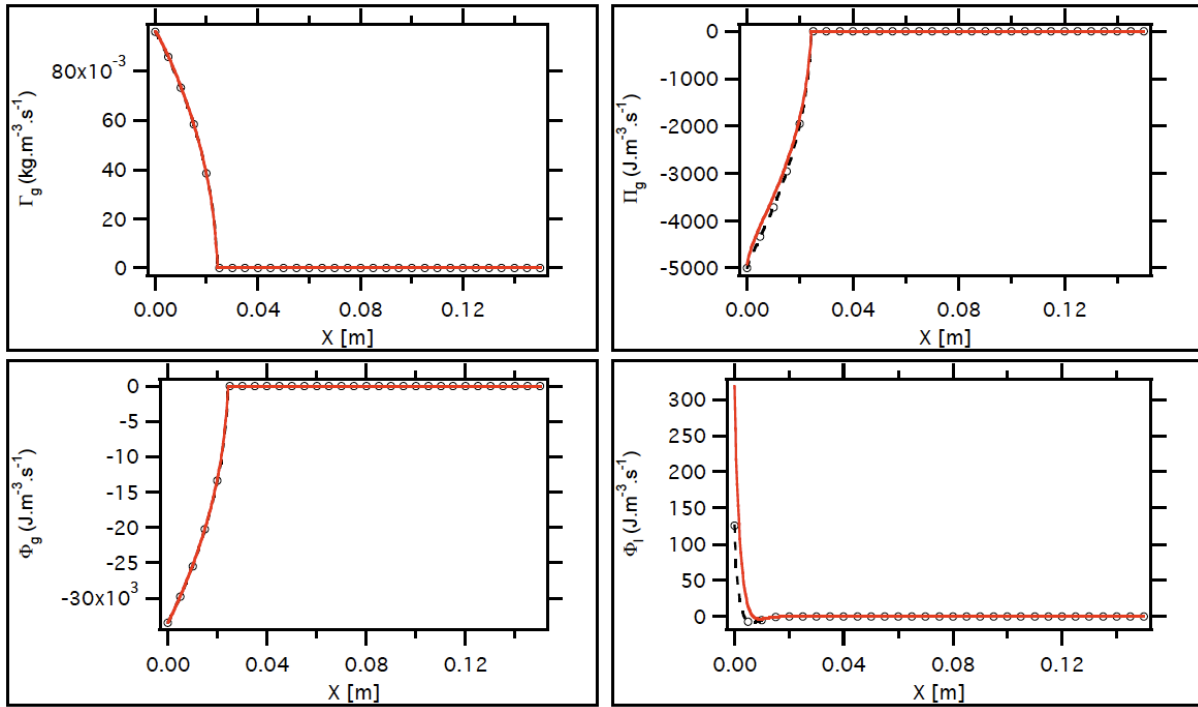


Figure 2: Comparison between EE AVBP_V6.1.4 tagged (-o-) and EE AVBP_V6.1.4 modified (—).

6.3 Comparison of results: EL AVBP_V6.1.4 tagged - EL AVBP_V6.1.4 modified

Figure 3 shows that the change in the reference temperature for the liquid enthalpy produce some differences in the calculation. While the mass source term (Γ_g) and the gaseous heat flux (Φ_g) show very small differences between the two calculations, the heat source term (Π_g) and the liquid heat flux (Φ_l) produce very different tendencies.

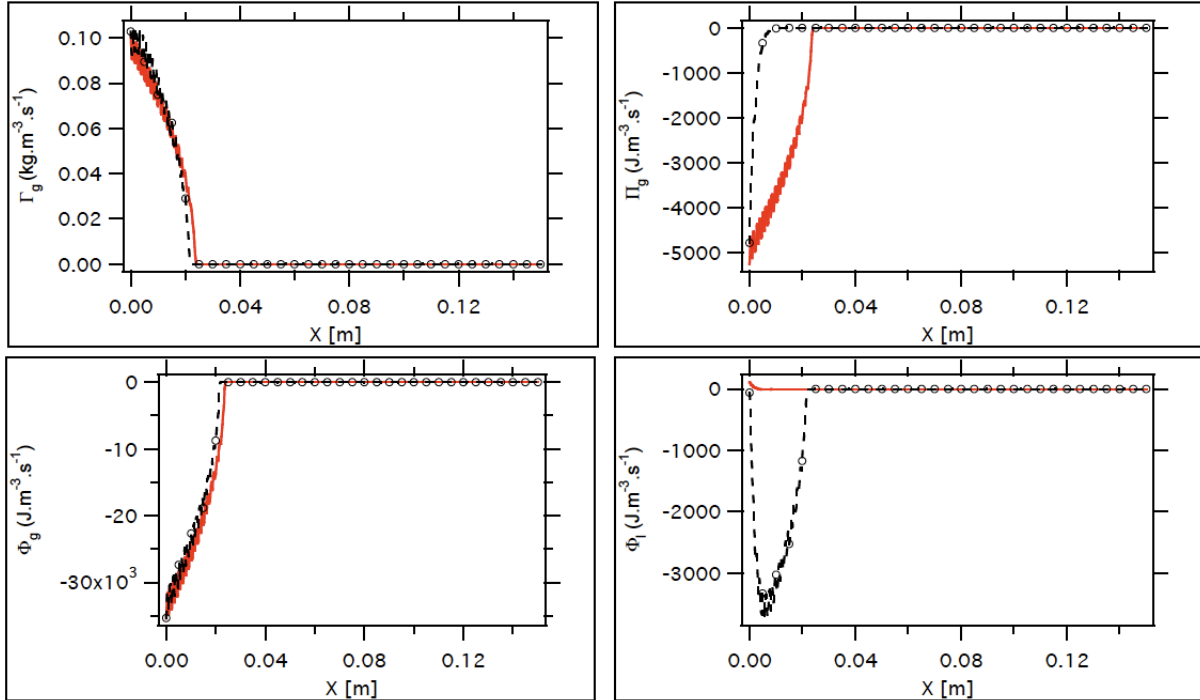


Figure 3: Comparison between EL AVBP_V6.1.4 tagged (—) and EL AVBP_V6.1.4 modified (-o-).

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