The ASTEC implementation of diffusion and settling

(presentation Porto Nov. 2006)

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Basic numerical scheme

$$\frac{\partial y_l}{\partial x} = f_l(x; z_i; t) \; , \qquad l = 1, \ldots I_1 \qquad \textbf{Type I}$$

$$\frac{\partial y_p}{\partial x} = f_p(x; z_i; t) + \sum_{i=1}^{I} \Lambda_{pi}(x; z_j; t) \frac{\partial y_i}{\partial t} \; , \qquad p = I_1 + 1, \ldots I_1 + I_2 \qquad \textbf{Type II}$$

$$\frac{\partial y_u}{\partial t} = f_u(x; z_i; t) \; , \qquad u = I_1 + I_2 + 1, \ldots I_1 + I_2 + I_3 \qquad \textbf{Type III}$$

$$y_i = y_i(x; z_j; t) \; , \qquad i = 1, \ldots I \; ,$$

$$g_\alpha(x_1; z_i(x_1); \lambda_k) = 0 \; , \qquad \alpha = 1, \ldots, KA \; ,$$

$$g_\beta(x_2; z_i(x_2); \lambda_k) = 0 \; , \qquad \beta = KA + 1, \ldots, KA + KB \; .$$

Subroutine tnrkt

Treatment of diffusion

Basic equation

$$\frac{\partial X_i}{\partial t} = \frac{\partial}{\partial m}\left(\mathcal{D}_i \frac{\partial X_i}{\partial m}\right) + \frac{\partial}{\partial m}(\mathcal{V}_i X_i) + \mathcal{R}_i \ ,$$

introduce

$$Y_i = \mathcal{D}_i \frac{\partial X_i}{\partial m} + \mathcal{V}_i X_i \ ;$$

Then

$$\begin{aligned} \frac{\partial X_i}{\partial m} &= \mathcal{D}_i^{-1} Y_i - \mathcal{D}_i^{-1} \mathcal{V}_i X_i \ , \\ \frac{\partial Y_i}{\partial m} &= \frac{\partial X_i}{\partial t} - \mathcal{R}_i \ , \end{aligned}$$

is on tnrkt form

Discretization

- Second-order spatially centred differences
- Time-centred differences in evolution equation for H
- Backwards differences for other elements, in general, and in energy equation (for stability)

Discretization, Type I

$$x_1 = x^1 < x^2 < \ldots x^n < x^{n+1} < \ldots < x^N = x_2$$

$$t = t^0, t^1, \ldots, t^s, t^{s+1}, \ldots$$

$$\frac{\partial y_l}{\partial x} = f_l(x; z_i; t) \ , \qquad l = 1, \ldots I_1$$

$$y_l^{n+1,s+1} - y_l^{n,s+1} = ½\Delta x^n (f_l^{n+1,s+1} + f_l^{n,s+1}), \qquad n = 1, \ldots, N-1; l = 1, \ldots, I1,$$

$$z_i^{n,s} = z_i(x^n, t^s)$$
$$y_i^{n,s} = y_i(x^n; z_j^{n,s}; t^s)$$
$$\Delta x^n = x^{n+1} - x^n$$

Discretization, Type II

$$\frac{\partial y_p}{\partial x} = f_p(x; z_i; t) + \sum_{i=1}^{I} \Lambda_{pi}(x; z_j; t) \frac{\partial y_i}{\partial t}, \qquad p = I_1 + 1, \ldots I_1 + I_2$$

$$\theta_p(y_p^{n+1,s+1} - y_p^{n,s+1}) + (1-\theta_p)(y_p^{n+1,s} - y_p^{n,s})$$
$$= \tfrac{1}{2}\Delta x^n \{\theta_p(f_p^{n+1,s+1} + f_p^{n,s+1}) + (1-\theta_p)(f_p^{n+1,s} + f_p^{n,s})$$
$$+ \sum_{i=1}^{I} [\theta_p \Lambda_{pi}^{n+1,s+1} + (1-\theta_p)\Lambda_{pi}^{n+1,s}] (z_i^{n+1,s+1} - z_i^{n+1,s})/\Delta t^s$$
$$+ \sum_{i=1}^{I} [\theta_p \Lambda_{pi}^{n,s+1} + (1-\theta_p)\Lambda_{pi}^{n,s}] (z_i^{n,s+1} - z_i^{n,s})/\Delta t^s\},$$
$$n = 1, \ldots, N-1; \qquad p = I1 + 1, \ldots, I1 + I2,$$

$$\Delta t^s = t^{s+1} - t^s$$

Discretization, Type III

$$\frac{\partial y_u}{\partial t} = f_u(x; z_i; t) \ , \qquad u = I_1 + I_2 + 1, \ldots I_1 + I_2 + I_3$$

$$y_u^{n,s+1} - y_u^{n,s} = \Delta t^s \left[\theta_u f_u^{n,s+1} + (1-\theta_u) f_u^{n,s}\right],$$

Note:

$\theta_u = 1$ for fully implicit (backwards) differences.

$\theta_u = 0.5$ for centred differences.

Implementation of diffusion

$$V_H = -\frac{B\,T^{5/2}}{\rho \ln\Lambda_{ij}(0.7+0.3X)} \left[\left(\frac{5}{4} + 1.125\nabla\right)(1-X)\frac{d\ln P}{dr} + \frac{(3+X)}{(1+X)(3+5X)}\frac{d\ln X}{dr}\right] \quad (17)$$

Hydrogen

$$V_i = -\frac{2BT^{5/2}}{5^{1/2}\rho Z_i^2}\left[\frac{\frac{d}{dr}\{\ln[\frac{X_i}{5X+3}(\frac{1+X}{5X+3})^{Z_i}]\} + [1+Z_i - A_i(\frac{5X+3}{4})]\frac{d\ln P}{dr}}{X(A_{ix}^{1/2}C_{ix} - A_{iy}^{1/2}C_{iy}) + A_{iy}^{1/2}C_{iy}}\right] + XV_H\frac{(A_{ix}^{1/2}C_{ix} - A_{iy}^{1/2}C_{iy})}{X(A_{ix}^{1/2}C_{ix} - A_{iy}^{1/2}C_{iy}) + A_{iy}^{1/2}C_{iy}} \quad (18)$$

Trace element

Represent all heavy elements by ^{16}O

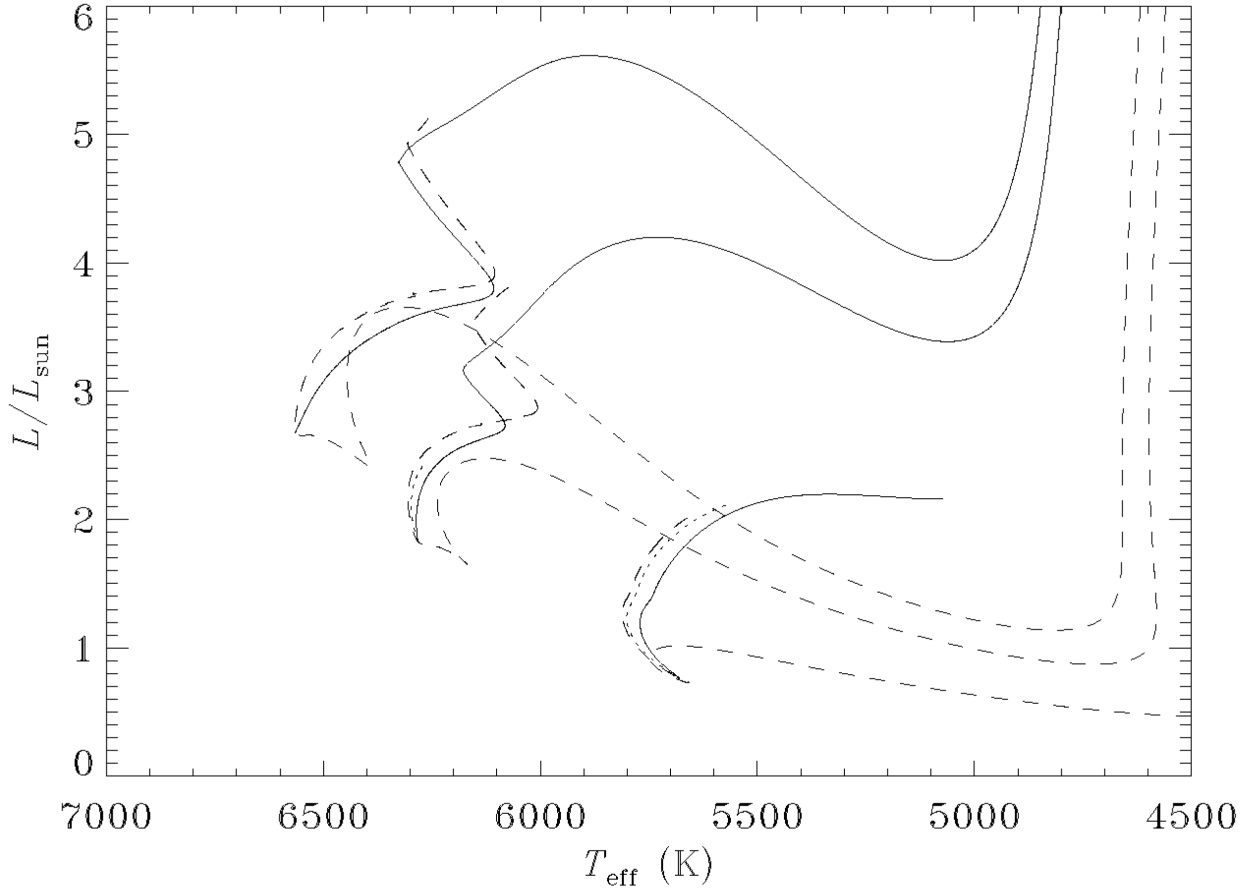
Michaud & Proffitt (1993: ASP Conf. Ser. 40, p. 246)

Comparison with CESAM(v1)

ASTEC (He)

ASTEC (He, Z)

CESAM



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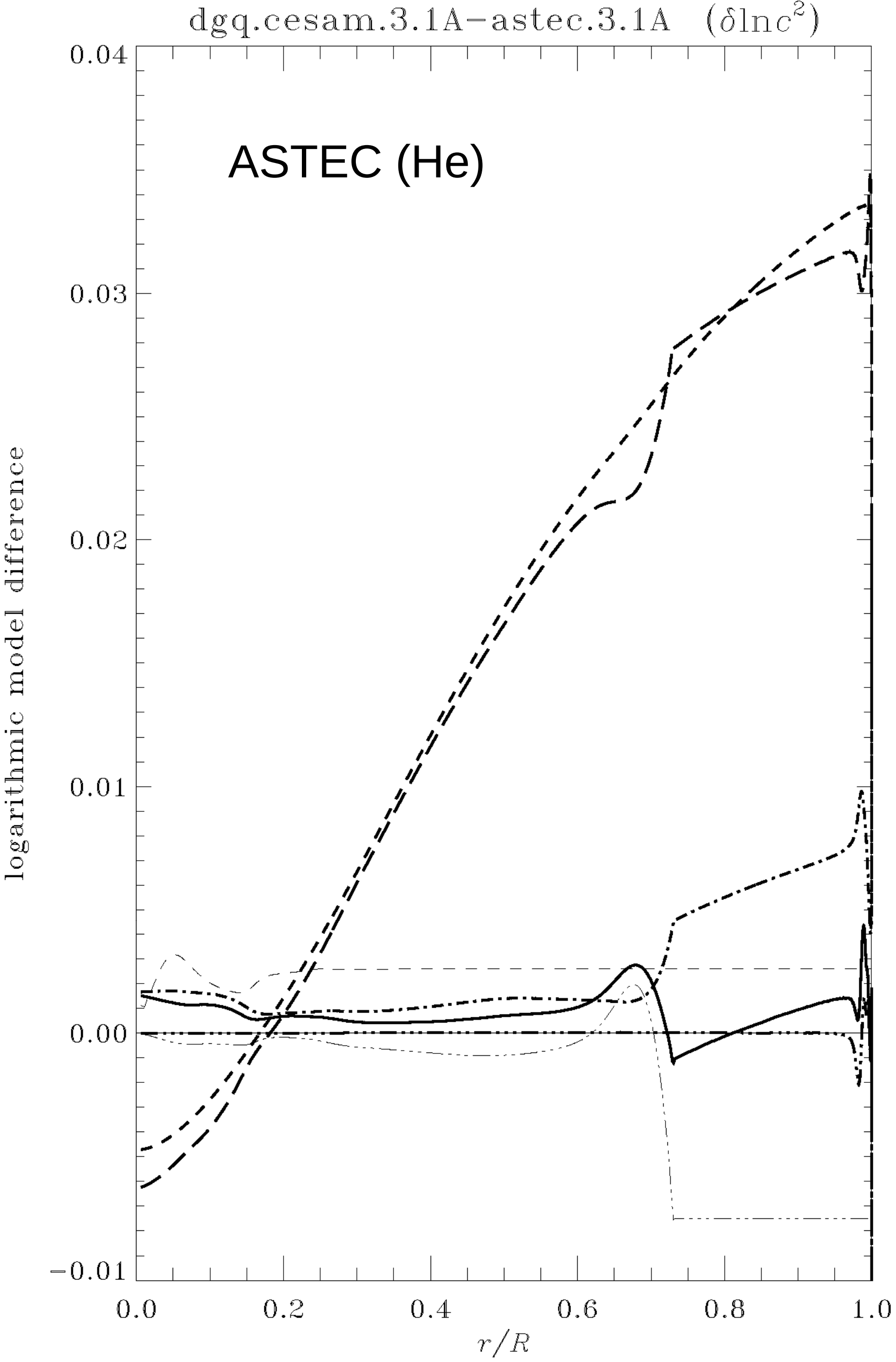

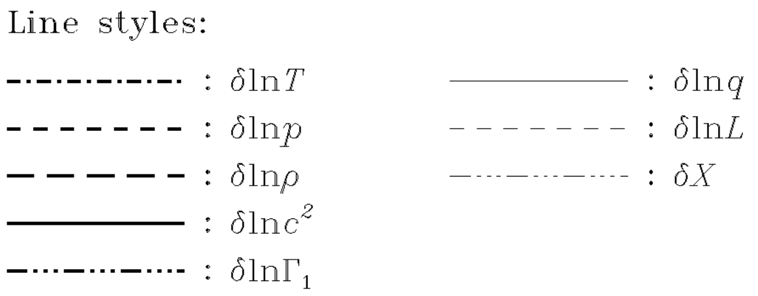

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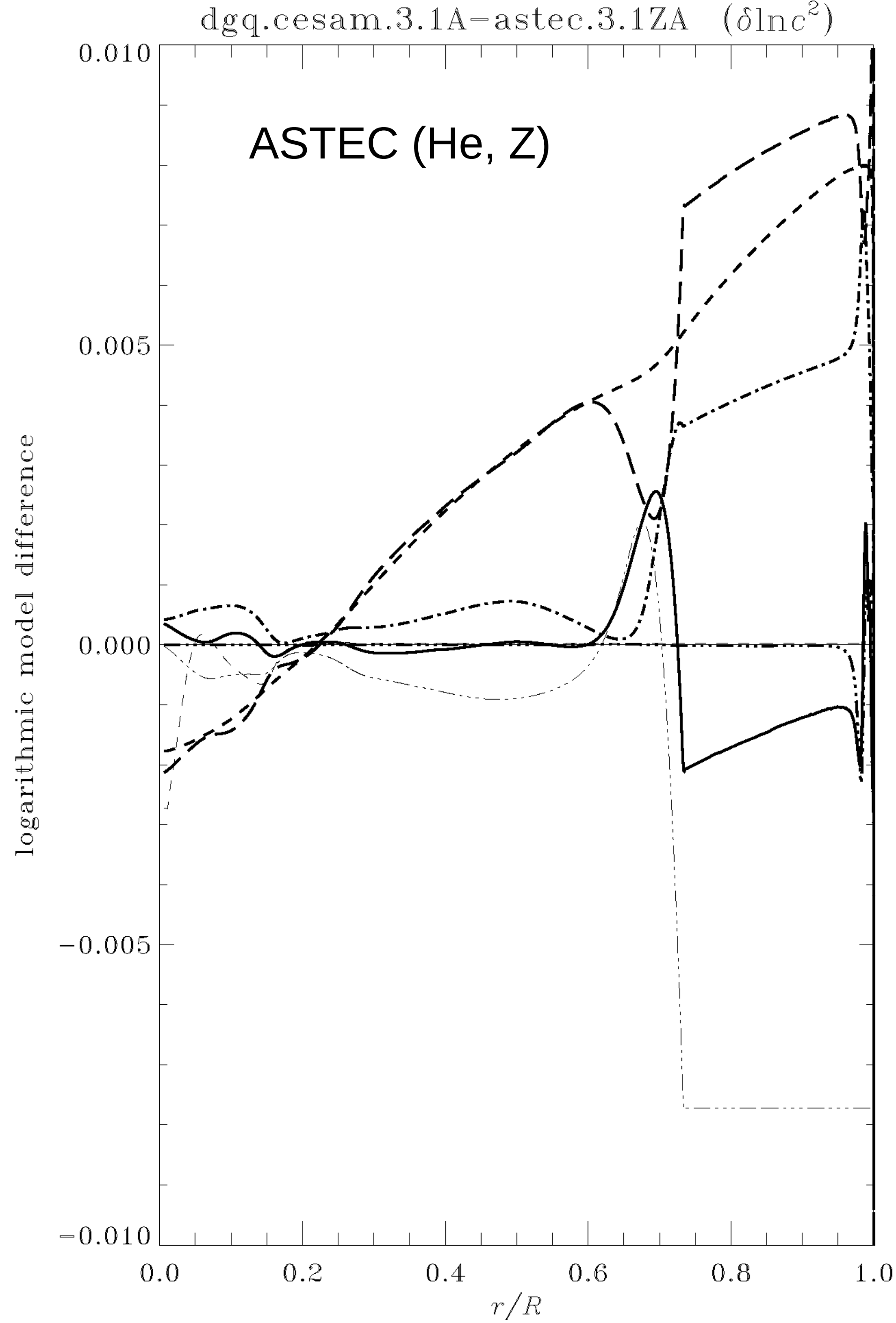

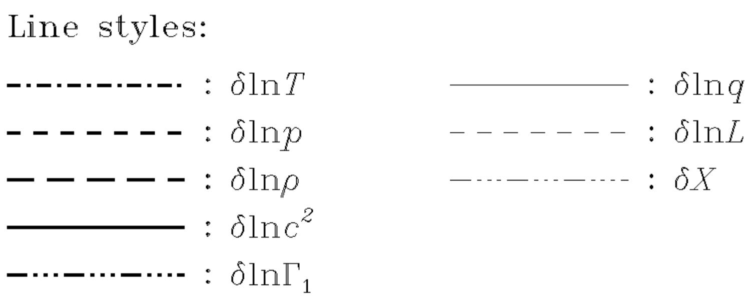

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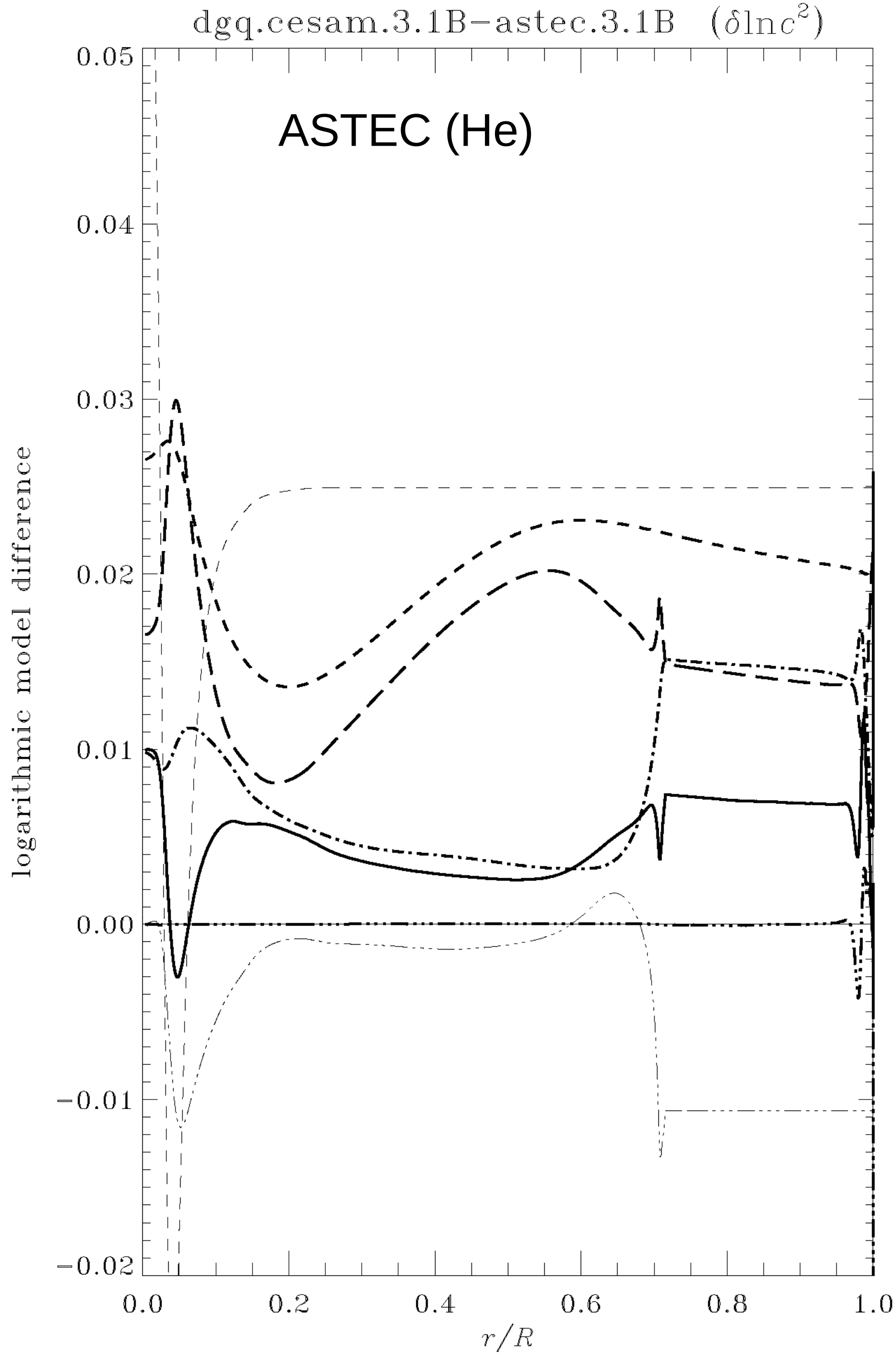

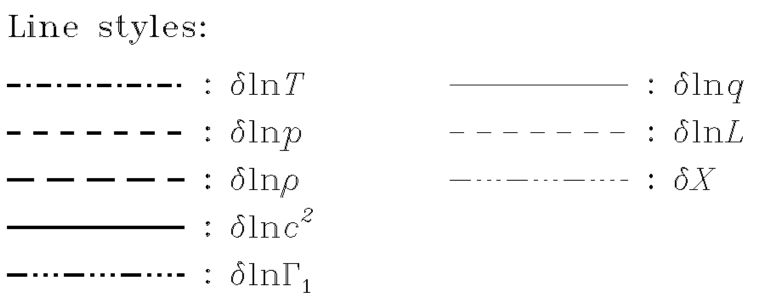

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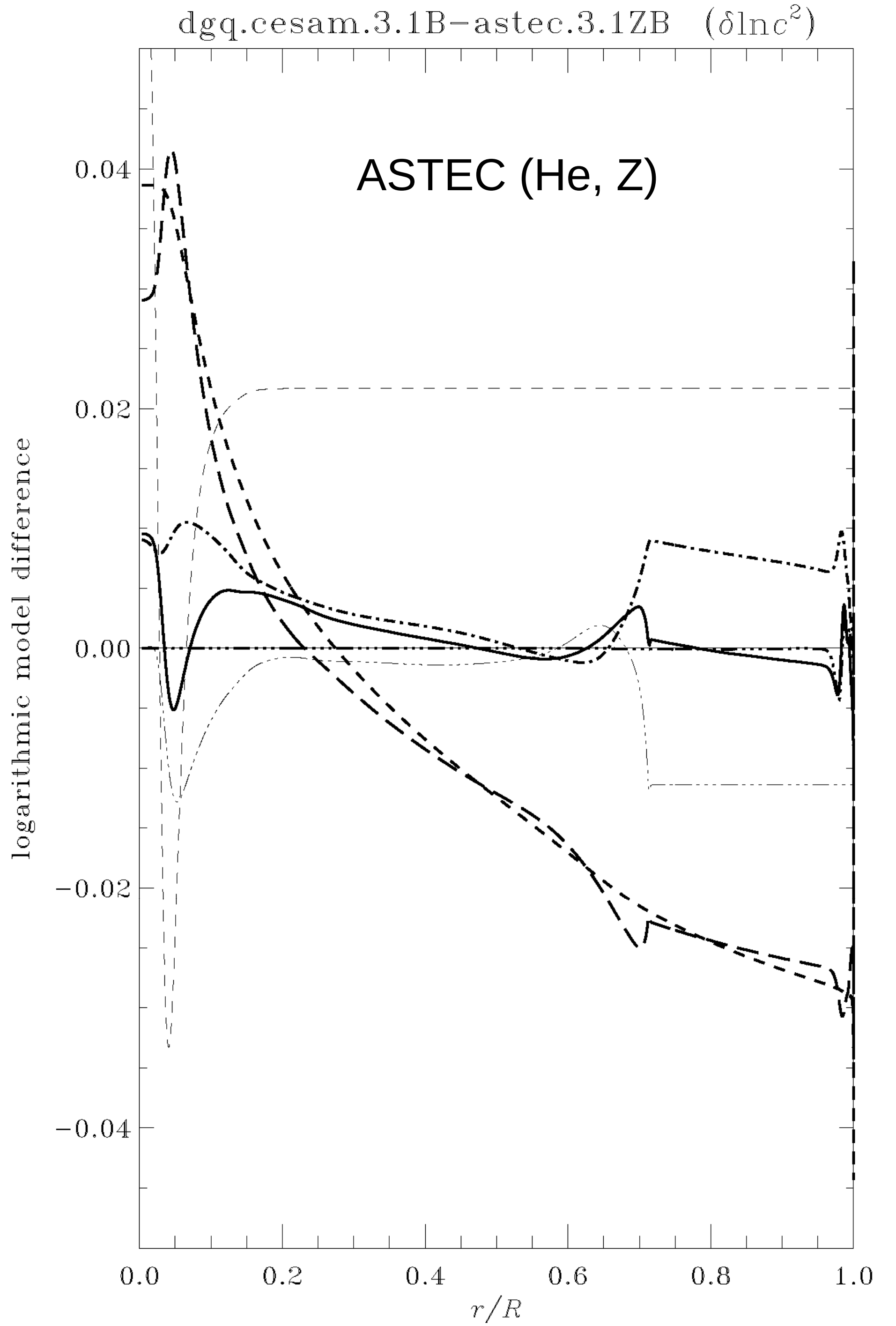

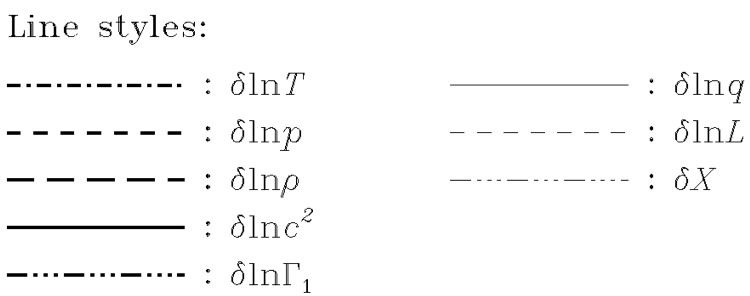

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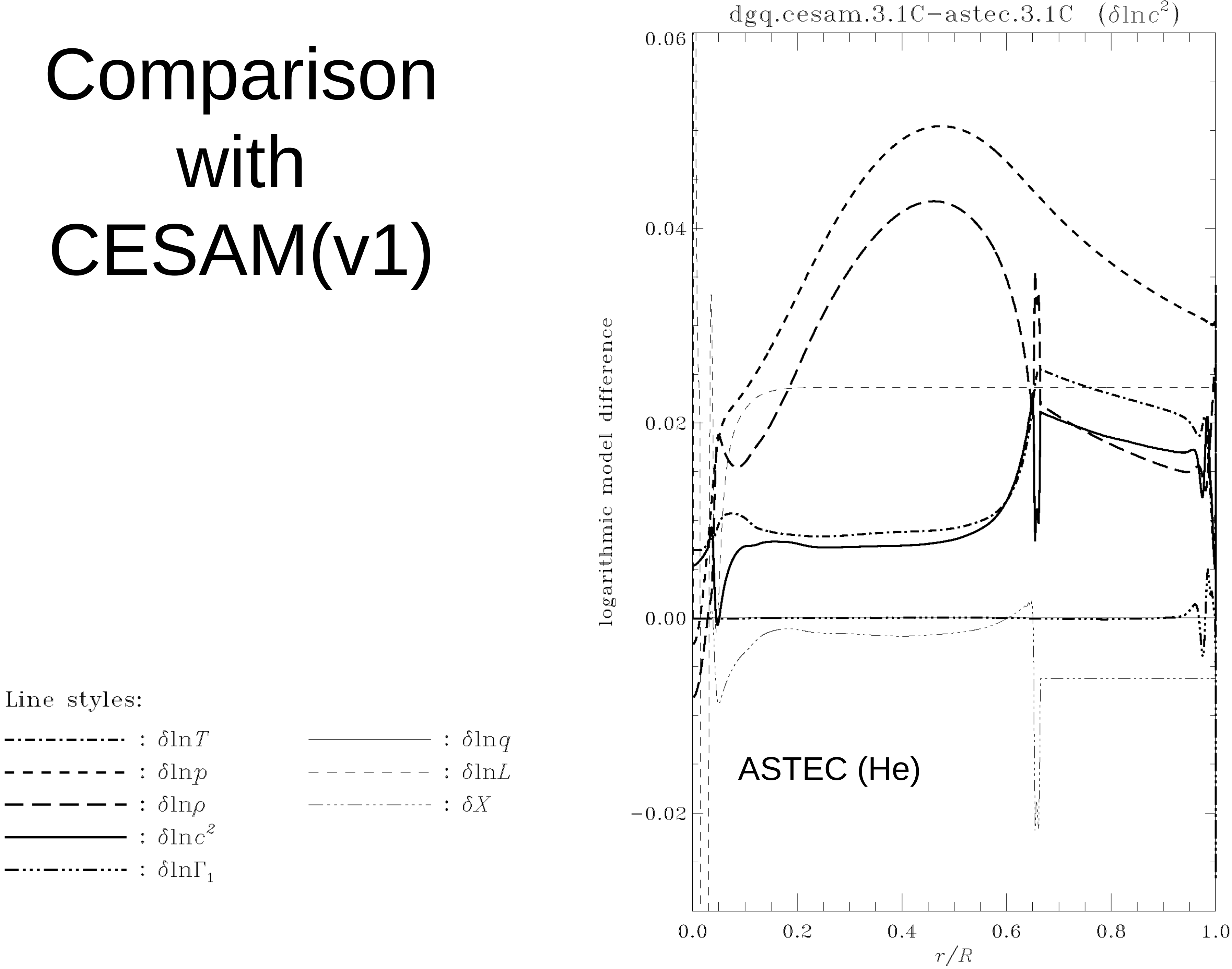

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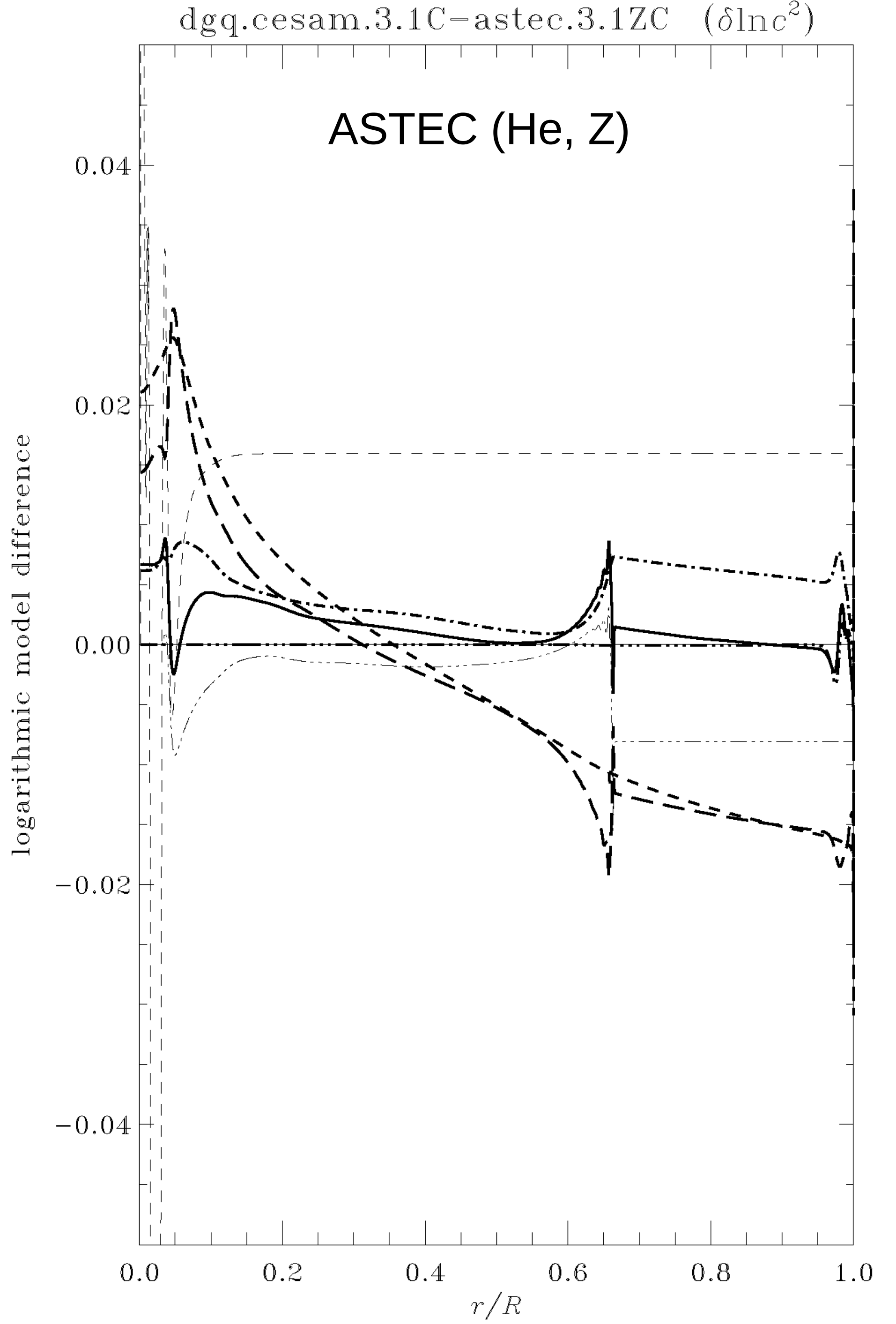
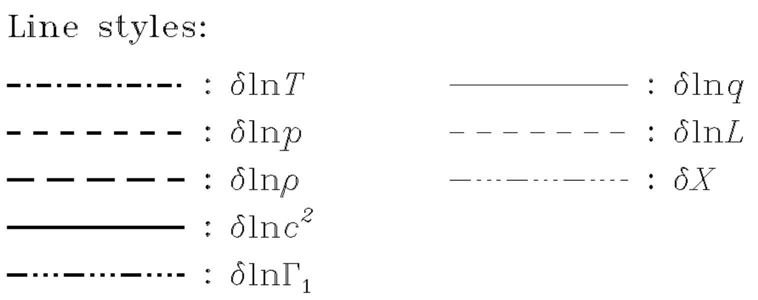
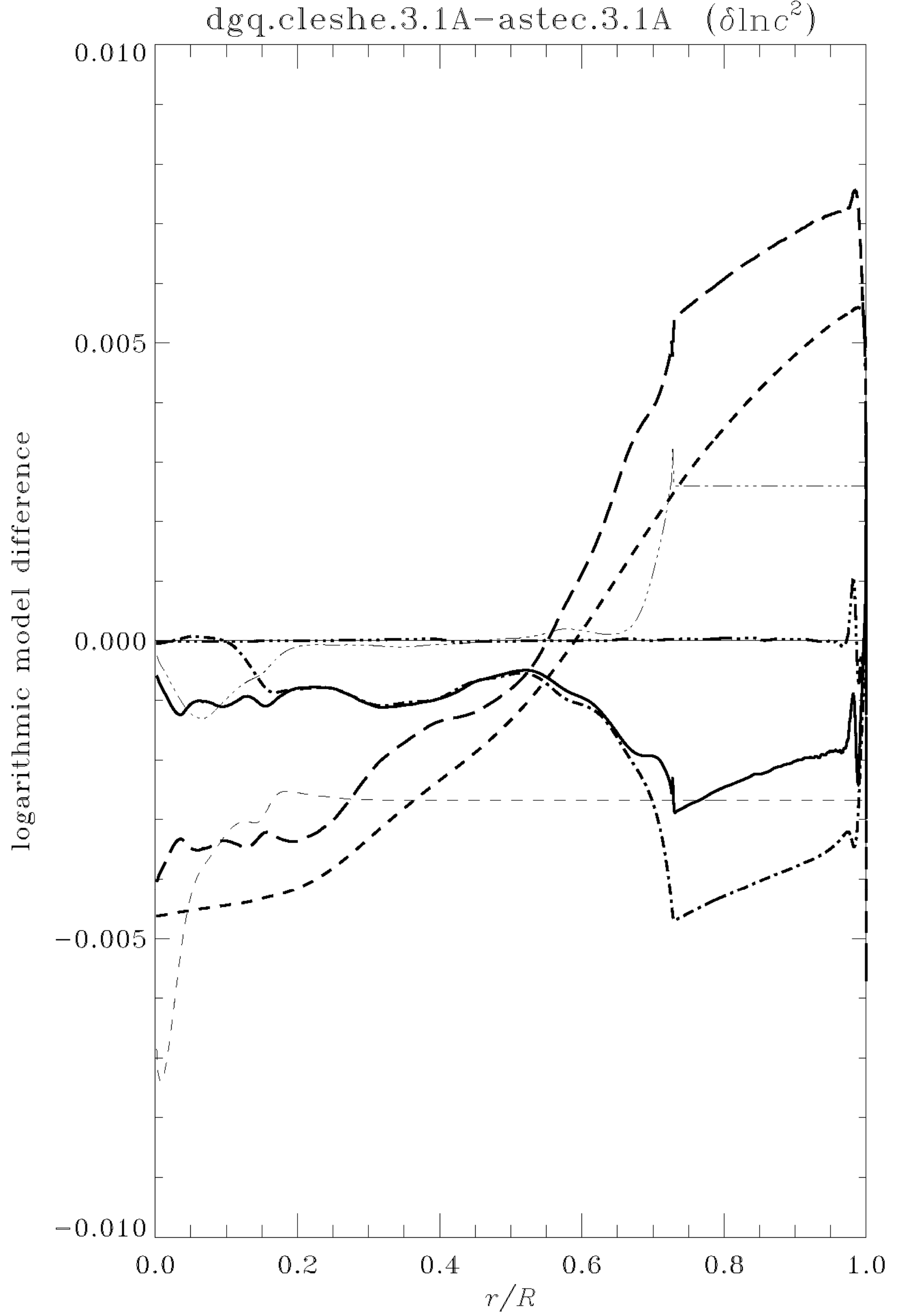
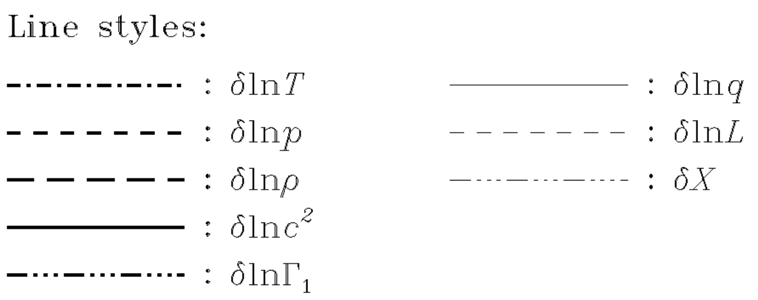




Comparison with CLES (He)





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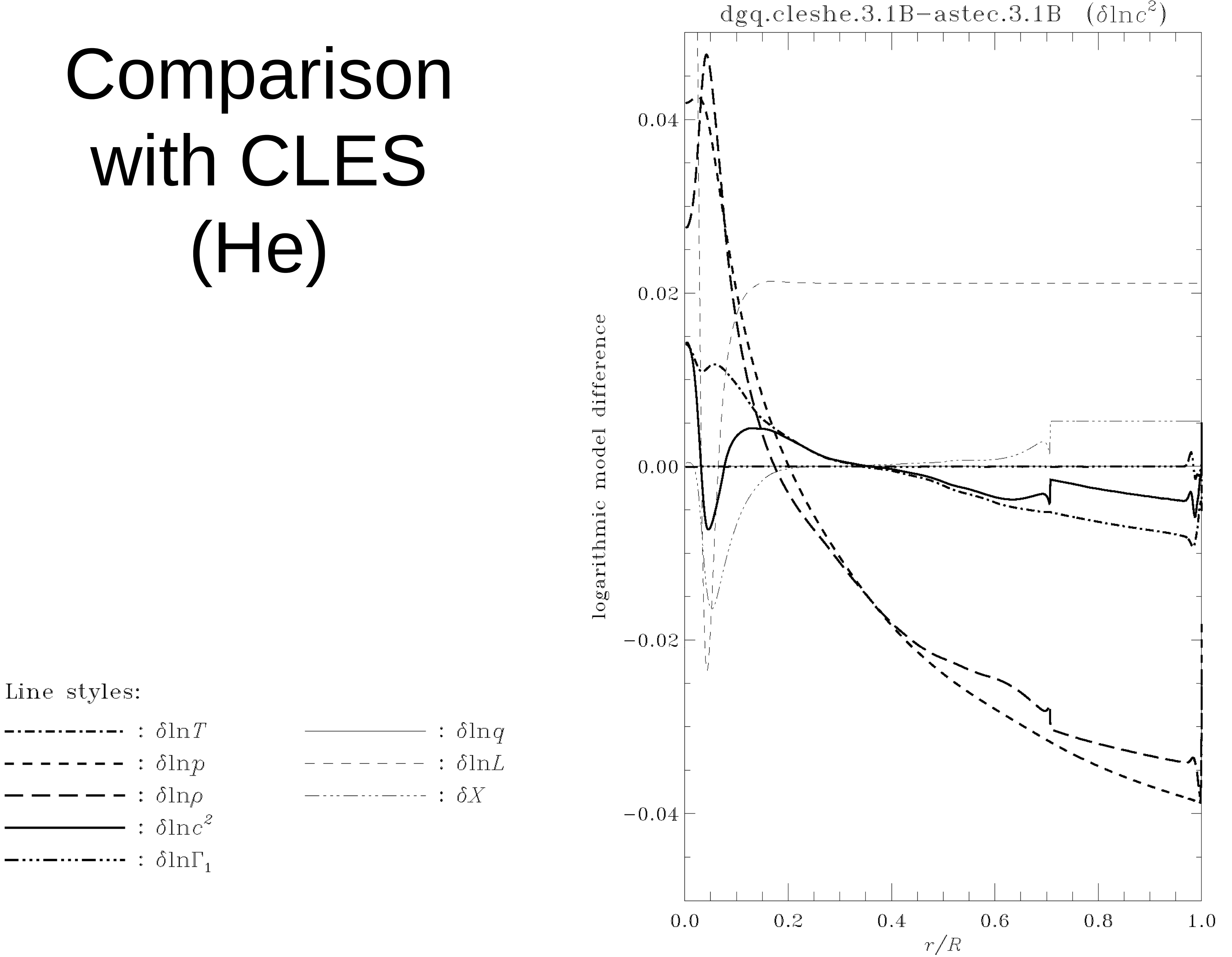

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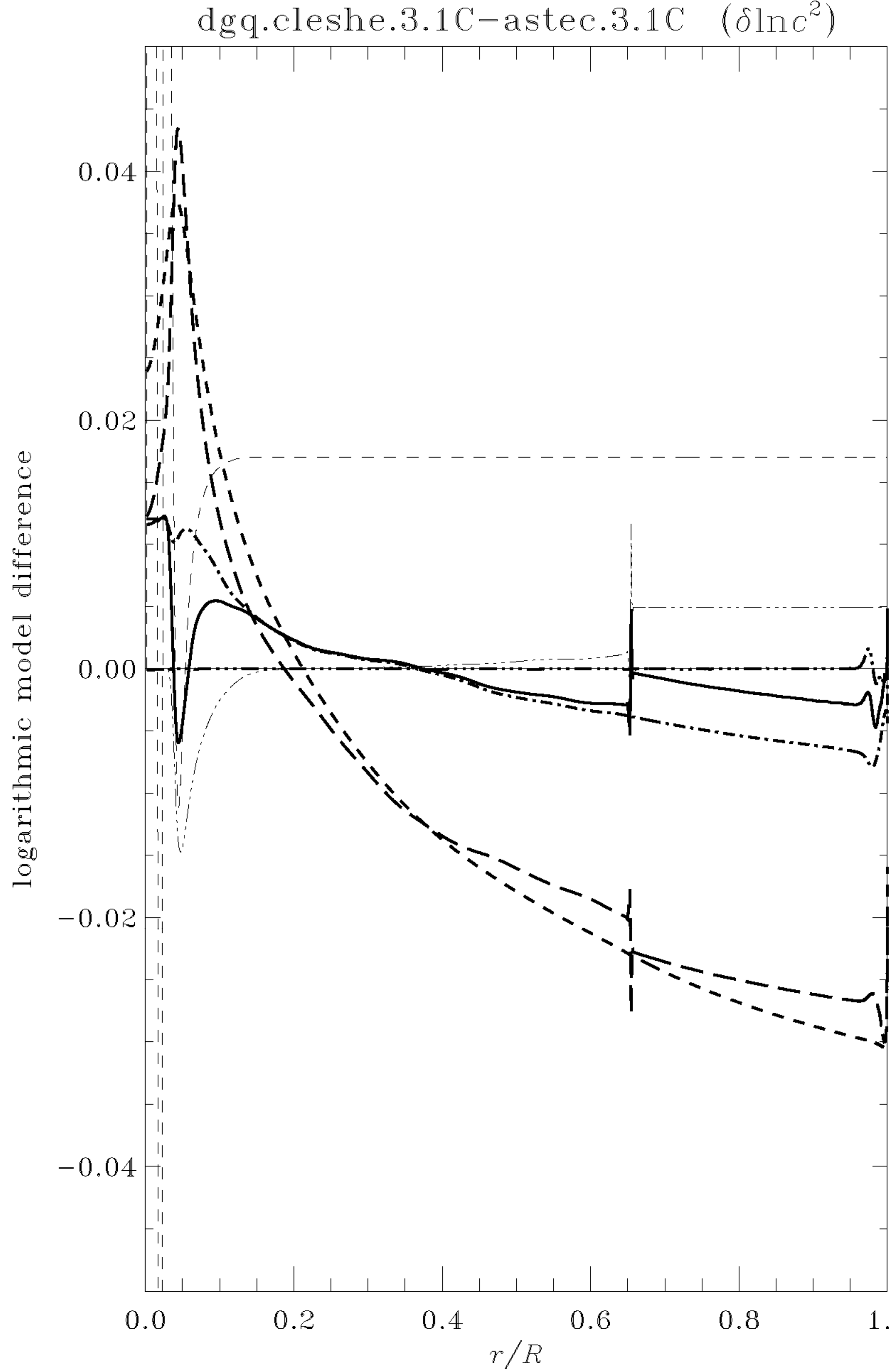

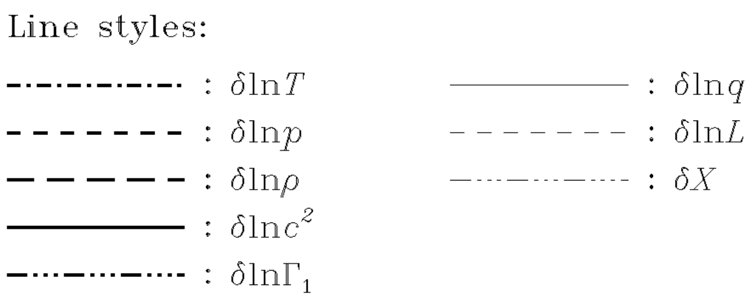

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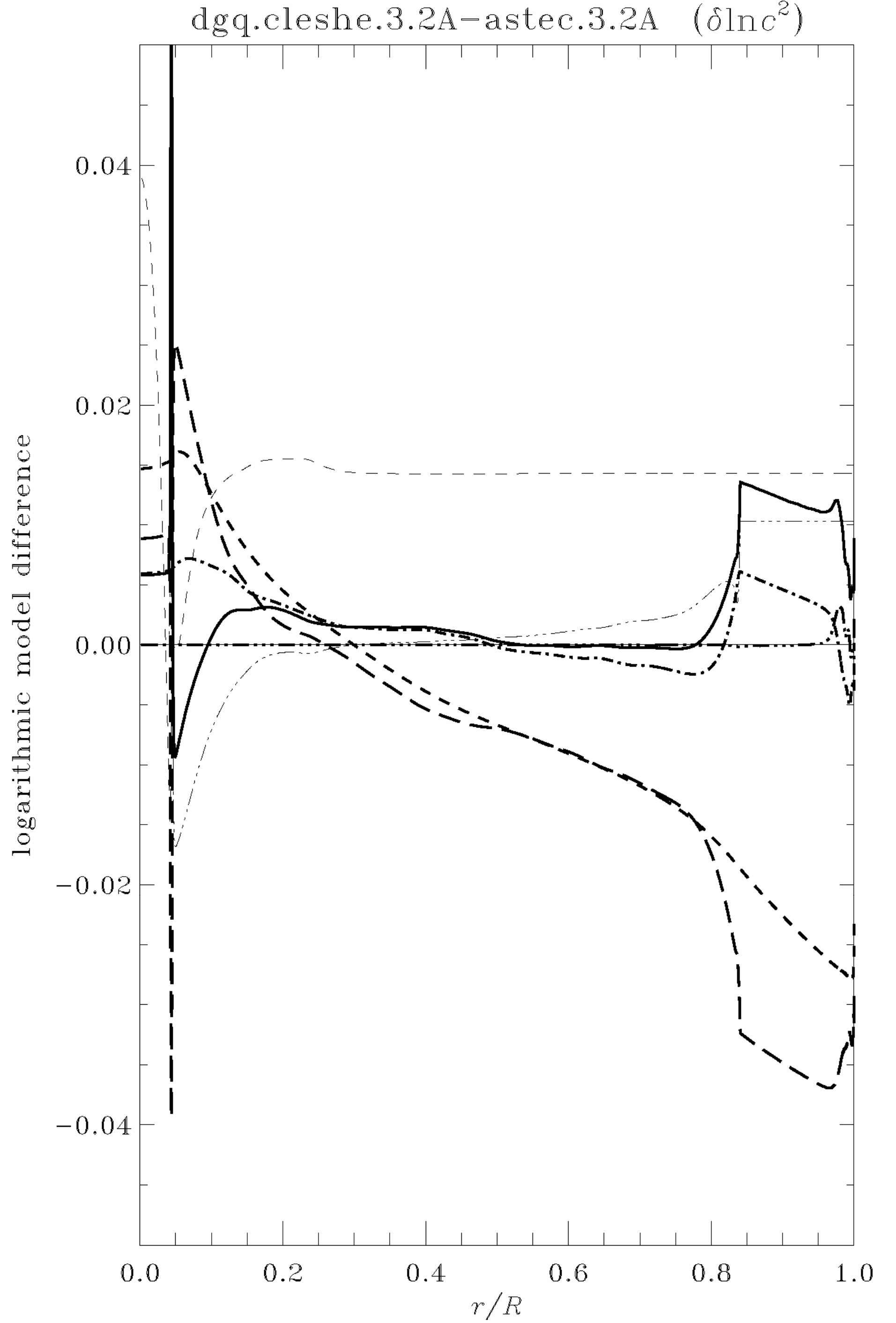
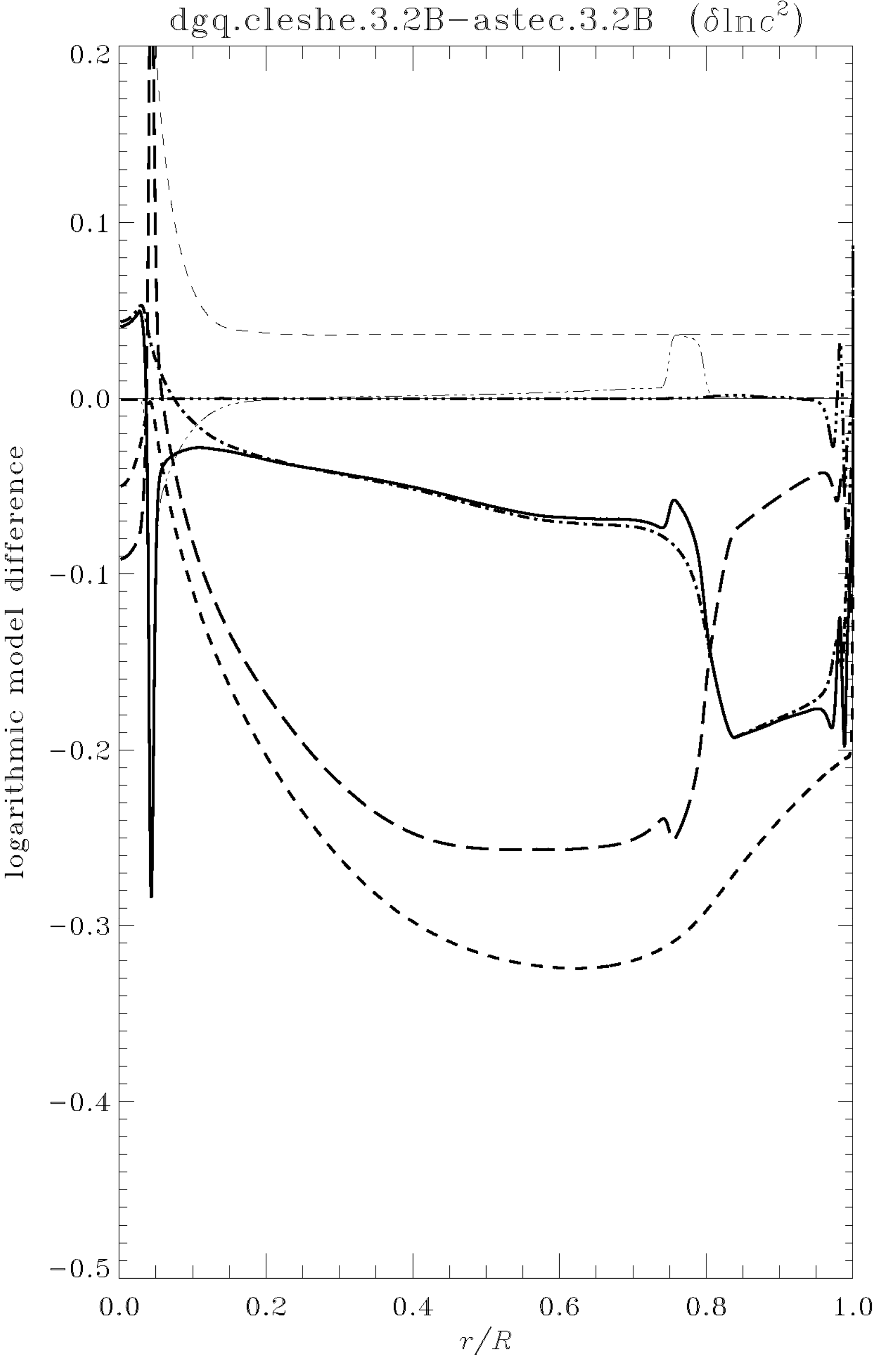
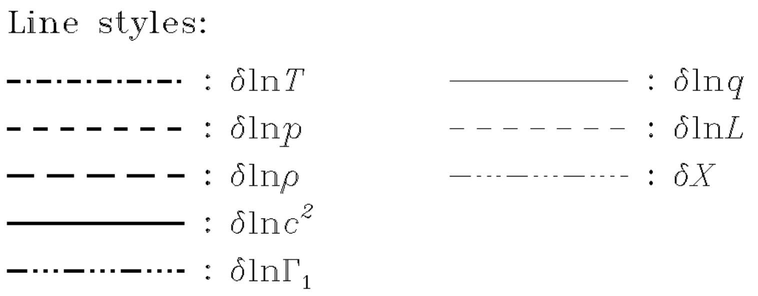


Line styles:

- : $\delta \ln T$
- : $\delta \ln p$
- : $\delta \ln \rho$
- : $\delta \ln c^2$
- : $\delta \ln \Gamma_1$
- : $\delta \ln q$
- : $\delta \ln L$
- : δX

Comparison with CLES (He)





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