An efficient kinetic modeling in plasmas by using the AWBS transport equation

Authors^{a,1}

^aCentre Lasers Intenses et Applications, Universite de Bordeaux-CNRS-CEA, UMR 5107, F-33405 Talence, France

Abstract

The AWBS Boltzmann transport equation for electrons equipped with a simplified e-e collision operator [?] provides an efficient, yet physically relevant, kinetic extension compared the classical Spitzer-Harm heat flux (SH) based on local approximation and flux-limiting. This classical approach is widely used in plasma kinetics models coupled to hydrodynamics. Even though SH reflects the electron-electron collision effect, the essential physical properties of the electron transport cannot be modeled with an explicitly local model. A simple form of the AWBS model opens a way to couple kinetics to hydrodynamic codes while describing the important physics correctly. Since the electron-electron collision effect becomes especially important in the case of low ion potential, we focus on presenting results related to low Z plasmas.

Keywords: kinetics; hydrodynamics; nonlocal electron transport; laser-heated plasmas.

E-mail address: milan.holec@u-bordeaux.fr

^{*}Corresponding author.

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7 1. Introduction

8 2. The AWBS nonlocal transport model

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f + \tilde{\boldsymbol{E}} \cdot \nabla_{\boldsymbol{v}} f = v \frac{\nu_e}{2} \frac{\partial}{\partial v} \left(f - f_M \right) + \frac{\nu_{ei} + \frac{\nu_e}{2}}{2} \frac{\partial^2 f}{\partial \boldsymbol{n}^2}, \tag{1}$$

19 [1]

3. BGK, AWBS, and Fokker-Planck models in diffusive regime

We can try to find an approximate solution while using the first term of expansion in λ_e and muas

$$\tilde{f}(z,v,\mu) = f^0(z,v) + f^1(z,v)\lambda_{ei}\mu. \tag{2}$$

 $_{23}$ 3.1. The BGK diffusive electron transport

$$\boldsymbol{n} \cdot \nabla f + \frac{1}{v} \left[\tilde{\boldsymbol{E}} \cdot \boldsymbol{n} \frac{\partial f}{\partial v} + \frac{\tilde{\boldsymbol{E}} \cdot \boldsymbol{e}_{\phi} - v \tilde{\boldsymbol{B}} \cdot \boldsymbol{e}_{\theta}}{v} \frac{\partial f}{\partial \phi} + \frac{\tilde{\boldsymbol{E}} \cdot \boldsymbol{e}_{\theta} + v \tilde{\boldsymbol{B}} \cdot \boldsymbol{e}_{\phi}}{v \sin(\phi)} \frac{\partial f}{\partial \theta} \right] = \frac{(f_M - f)}{\lambda^e} + \frac{1}{2\lambda^{ei}} \left(\frac{\partial}{\partial \mu} \left((1 - \mu^2) \frac{\partial f}{\partial \mu} \right) + \frac{1}{\sin^2(\phi)} \frac{\partial^2 f}{\partial \theta^2} \right), \quad (3)$$

where $\mu = \cos(\phi)$, λ_e is the electron-electron mean free path, and λ_{ei} is the electron-ion mean free path. We also approximate $\lambda_e = \bar{Z}\lambda_{ei}$.

Clearly, $\frac{\partial \tilde{f}}{\partial \theta} = 0$, and if $\tilde{\boldsymbol{E}} = \tilde{B}_z \boldsymbol{e}_z$, there is no effect of magnetic field. We also assume, that $\nabla f = \frac{\partial f}{\partial z} \boldsymbol{e}_z$ and appropriately $\tilde{\boldsymbol{E}} = \tilde{E}_z \boldsymbol{e}_z$. From the orientation of the Cartesian basis vectors and spherical basis vectors, one can find $\tilde{\boldsymbol{E}} \cdot \boldsymbol{n} = \tilde{E}_z \cos(\phi) = \mu$ and $\tilde{\boldsymbol{E}} \cdot \boldsymbol{e}_\phi = -\tilde{E}_z \sin(\phi)$. As a result, the analyzed BGK equation reads

$$\mu \frac{\partial}{\partial z} \left(f^{0} + f^{1} \lambda_{ei} \mu \right) + \frac{1}{v} \left[\tilde{E}_{z} \mu \frac{\partial}{\partial v} \left(f^{0} + f^{1} \lambda_{ei} \mu \right) - \frac{\tilde{E}_{z} \sin(\phi)}{v} \frac{\partial}{\partial \phi} \left(f^{0} + f^{1} \lambda_{ei} \mu \right) \right] = \frac{(f_{M} - (f^{0} + f^{1} \lambda_{ei} \mu))}{\lambda_{e}} + \frac{1}{2\lambda_{ei}} \frac{\partial}{\partial \mu} \left((1 - \mu^{2}) \frac{\partial}{\partial \mu} \left(f^{0} + f^{1} \lambda_{ei} \mu \right) \right), \quad (4)$$

$$\mu \frac{\partial f^{0}}{\partial z} + \mu^{2} \frac{\partial}{\partial z} \left(f^{1} \lambda_{ei} \right) + \frac{\tilde{E}_{z}}{v} \left[\mu \frac{\partial f^{0}}{\partial v} + \mu^{2} \frac{\partial}{\partial v} \left(f^{1} \lambda_{ei} \right) + \frac{1 - \mu^{2}}{v} f^{1} \lambda_{ei} \right] = \frac{f_{M} - f^{0}}{\bar{Z} \lambda_{ei}} - \mu \frac{1}{\bar{Z}} f^{1} - \mu f^{1}, \quad (5)$$

consequently, we have the following anisotropy expansion $\mu^0, \mu^1, \mu^2, ...$ equations

$$\frac{f_M - f^0}{\bar{Z}\lambda_{ei}} = \frac{E_z}{v^2} f^1 \lambda_{ei},$$

$$\frac{\partial f^0}{\partial z} + \frac{\tilde{E}_z}{v} \frac{\partial f^0}{\partial v} = -\frac{1}{\bar{Z}} f^1 - f^1,$$

$$\frac{\partial}{\partial z} \left(f^1 \lambda_{ei} \right) + \frac{\tilde{E}_z}{v} \left[\frac{\partial}{\partial v} \left(f^1 \lambda_{ei} \right) - \frac{1}{v} f^1 \lambda_{ei} \right] = 0,$$

which lead to the definitions

$$f^{0} = f_{M} + \frac{1}{v} f^{1} \bar{Z} \lambda_{ei}^{2},$$

$$f^{1} = -\frac{\bar{Z}}{\bar{Z} + 1} \left[\frac{\partial f^{0}}{\partial z} + \frac{\tilde{E}_{z}}{v} \frac{\partial f^{0}}{\partial v} \right]$$

$$= -\frac{\bar{Z}}{\bar{Z} + 1} \left[\frac{1}{\rho} \frac{\partial \rho}{\partial z} + \left(\frac{v^{2}}{2v_{th}^{2}} - \frac{3}{2} \right) \frac{1}{T} \frac{\partial T}{\partial z} - \frac{\tilde{E}_{z}}{v_{th}^{2}} \right] f_{M}$$

$$(6)$$

In order to ensure the plasma to be quasi-neutral, the zero-current condition

$$\mathbf{j} = \int_0^\infty \int_{4\pi} q_e v \mathbf{n} f \, d\mathbf{n} \ v^2 \, dv = \mathbf{0}, \tag{8}$$

can be achieved by providing a consistent electric field in (15), i.e.

$$\tilde{\boldsymbol{E}} = \frac{v_{th}^2 \int_{4\pi} \boldsymbol{n} \otimes \boldsymbol{n} \cdot \int_0^\infty v f_M \frac{\lambda}{\alpha} \left(\frac{\nabla \rho}{\rho} + \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} \right) \frac{\nabla T}{T} \right) v^2 \, dv \, d\boldsymbol{n}}{\int_{4\pi} \boldsymbol{n} \otimes \boldsymbol{n} \cdot \int_0^\infty v f_M \frac{\lambda}{\alpha} v^2 \, dv \, d\boldsymbol{n}}, \quad (9)$$

which may be further simplified as

$$\tilde{\boldsymbol{E}} = \frac{\int_0^\infty f_M \frac{1}{2} \frac{\nabla T}{T} v^9 \, \mathrm{d}v}{\int_0^\infty f_M v^7 \, \mathrm{d}v} + v_{th}^2 \left(\frac{\nabla \rho}{\rho} - \frac{3}{2} \frac{\nabla T}{T}\right) = v_{th}^2 \left(\frac{\nabla \rho}{\rho} + \frac{5}{2} \frac{\nabla T}{T}\right), \quad (10)$$

where it is worth mentioning, that the part $f_M + \frac{v\lambda}{\alpha} \frac{\partial f_1}{\partial v}$ of the distribution does not contribute to the current since it is isotropic. One can write the quasineutral distribution function explicitly distinguishing between original part (blue color) and E field correction (red color) as

$$f \approx f_M \left(1 - \frac{\lambda}{\alpha} \boldsymbol{n} \cdot \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} - \frac{5}{2} \right) \frac{\nabla T}{T} \right) + \frac{v\lambda}{\alpha} \frac{\partial f_1}{\partial v}.$$
 (11)

which leads to the resulting heat flux

$$\boldsymbol{q}_{H} = \int_{4\pi} \int_{0}^{\infty} \frac{m_{e}v^{2}}{2} v \boldsymbol{n} f v^{2} \, \mathrm{d}v \, \mathrm{d}\boldsymbol{n} = \frac{4\pi}{3} \frac{m_{e}}{2} \frac{1}{\alpha \sigma \rho} \int_{0}^{\infty} \left(\frac{v^{2}}{2v_{th}^{2}} - \frac{3}{2} - \frac{5}{2} \right) v^{9} f_{M} \, \mathrm{d}v \frac{\nabla T}{T}.$$

Based on the Gauss integral formula

$$\int v^{2s+1} \exp\left(-\frac{v^2}{2v_{th}^2}\right) dv = \frac{s! (2v_{th}^2)^{s+1}}{2}$$

and Maxwell-Boltzmann distribution (??) the heat flux can be written as

$$\boldsymbol{q}_{H} = \frac{4\pi}{3} \frac{m_{e}}{2} \frac{1}{\alpha \sigma \rho} \frac{\rho}{v_{th}^{3} (2\pi)^{3/2}} \frac{4! \ 2^{4} v_{th}^{10}}{T} \left(5 - \frac{3}{2} - \frac{5}{2}\right) \nabla T = \frac{m_{e}}{\alpha \sigma} \frac{128}{\sqrt{2\pi}} \left(\frac{k_{B}}{m_{e}}\right)^{\frac{7}{2}} T^{\frac{5}{2}} \nabla T.$$

$$(12)$$

In conclusion, equation (12) provides nothing else than the well known Lorentz

41 approximation heat flux and its nonlinearity 2.5 in temperature. What is

worth mentioning is the effect of E field (quasi-neutrality), which reduces

the flux of about 71.4% (also assuming constant density).

Finally, one can find the approximate solution

$$\tilde{f} = f_M - \lambda_{ei} \frac{\bar{Z}}{\bar{Z} + 1} \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} - \alpha \right) \frac{\boldsymbol{n} \cdot \nabla T}{T} f_M. \tag{13}$$

3.2. The AWBS diffusive electron transport

The AWBS electron transport equation in 6D reads

$$\boldsymbol{n} \cdot \nabla f + \frac{1}{v} \left[\tilde{\boldsymbol{E}} \cdot \boldsymbol{n} \frac{\partial f}{\partial v} + \frac{\tilde{\boldsymbol{E}} \cdot \boldsymbol{e}_{\phi} - v \tilde{\boldsymbol{B}} \cdot \boldsymbol{e}_{\theta}}{v} \frac{\partial f}{\partial \phi} + \frac{\tilde{\boldsymbol{E}} \cdot \boldsymbol{e}_{\theta} + v \tilde{\boldsymbol{B}} \cdot \boldsymbol{e}_{\phi}}{v \sin(\phi)} \frac{\partial f}{\partial \theta} \right] = \frac{v}{\lambda^{e}} \frac{\partial}{\partial v} \left(f - f_{M} \right) + \left(\frac{1}{\lambda_{ei}} + \frac{1}{\lambda_{e}} \right) \frac{1}{2} \left(\frac{\partial}{\partial \mu} \left((1 - \mu^{2}) \frac{\partial f}{\partial \mu} \right) + \frac{1}{\sin^{2}(\phi)} \frac{\partial^{2} f}{\partial \theta^{2}} \right), \quad (14)$$

where $\mu = \cos(\phi)$, λ_e is the electron-electron mean free path, and λ_{ei} is the electron-ion mean free path, and $\lambda_e = \bar{Z}\lambda_{ei}$.

We can try to find an approximate solution while using the first term of expansion in λ_e and μ as

$$\tilde{f}(z,v,\mu) = f^0(z,v) + f^1(z,v)\lambda_{ei}\mu. \tag{15}$$

Clearly, $\frac{\partial \tilde{f}}{\partial \theta} = 0$, and if $\tilde{\boldsymbol{E}} = \tilde{B}_z \boldsymbol{e}_z$, there is no effect of magnetic field. We also assume, that $\nabla f = \frac{\partial f}{\partial z} \boldsymbol{e}_z$ and appropriately $\tilde{\boldsymbol{E}} = \tilde{E}_z \boldsymbol{e}_z$. From the orientation of the Cartesian basis vectors and spherical basis vectors, one can find $\tilde{\boldsymbol{E}} \cdot \boldsymbol{n} = \tilde{E}_z \cos(\phi) = \mu$ and $\tilde{\boldsymbol{E}} \cdot \boldsymbol{e}_\phi = -\tilde{E}_z \sin(\phi)$. As a result, the analyzed AWBS equation reads

$$\mu \frac{\partial}{\partial z} \left(f^{0} + f^{1} \lambda_{ei} \mu \right) + \frac{1}{v} \left[\tilde{E}_{z} \mu \frac{\partial}{\partial v} \left(f^{0} + f^{1} \lambda_{ei} \mu \right) - \frac{\tilde{E}_{z} \sin(\phi)}{v} \frac{\partial}{\partial \phi} \left(f^{0} + f^{1} \lambda_{ei} \mu \right) \right] = \frac{v}{\lambda_{e}} \frac{\partial}{\partial v} \left(\left(f^{0} + f^{1} \lambda_{ei} \mu \right) - f_{M} \right) + \frac{\bar{Z} + 1}{2\lambda_{ei} \bar{Z}} \frac{\partial}{\partial \mu} \left((1 - \mu^{2}) \frac{\partial}{\partial \mu} \left(f^{0} + f^{1} \lambda_{ei} \mu \right) \right), \tag{16}$$

$$\mu \frac{\partial f^{0}}{\partial z} + \mu^{2} \frac{\partial}{\partial z} \left(f^{1} \lambda_{ei} \right) + \frac{\tilde{E}_{z}}{v} \left[\mu \frac{\partial f^{0}}{\partial v} + \mu^{2} \frac{\partial}{\partial v} \left(f^{1} \lambda_{ei} \right) + \frac{1 - \mu^{2}}{v} f^{1} \lambda_{ei} \right] = \frac{v}{\bar{Z} \lambda_{ei}} \frac{\partial}{\partial v} \left(f^{0} - f_{M} \right) + \mu \frac{v}{\bar{Z} \lambda_{ei}} \frac{\partial (f^{1} \lambda_{ei})}{\partial v} - \mu \frac{\bar{Z} + 1}{\bar{Z}} f^{1}, \quad (17)$$

consequently, we have the following anisotropy expansion $\mu^0, \mu^1, \mu^2, ...$ equations

$$\frac{v}{\bar{Z}\lambda_{ei}}\frac{\partial}{\partial v}\left(f^{0}-f_{M}\right) = \frac{\tilde{E}_{z}}{v^{2}}f^{1}\lambda_{ei},$$

$$\frac{\partial f^{0}}{\partial z} + \frac{\tilde{E}_{z}}{v}\frac{\partial f^{0}}{\partial v} = \frac{v}{\bar{Z}\lambda_{ei}}\frac{\partial(f^{1}\lambda_{ei})}{\partial v} - \frac{\bar{Z}+1}{\bar{Z}}f^{1},$$

$$\frac{\partial}{\partial z}\left(f^{1}\lambda_{ei}\right) + \frac{\tilde{E}_{z}}{v}\left[\frac{\partial}{\partial v}\left(f^{1}\lambda_{ei}\right) - \frac{1}{v}f^{1}\lambda_{ei}\right] = 0,$$

52 which lead to the definitions

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56

$$\frac{\partial}{\partial v} \left(f^{0} - f_{M} \right) = \frac{1}{v^{2}} f^{1} \bar{Z} \lambda_{ei}^{2}, \tag{18}$$

$$\frac{v}{\bar{Z} \lambda_{ei}} \frac{\partial (f^{1} \lambda_{ei})}{\partial v} - \frac{\bar{Z} + 1}{\bar{Z}} f^{1} = \frac{\partial f^{0}}{\partial z} + \frac{\tilde{E}_{z}}{v} \frac{\partial f^{0}}{\partial v}$$

$$\frac{v}{\bar{Z}} \frac{\partial f^{1}}{\partial v} + \frac{4}{\bar{Z}} f^{1} - \frac{\bar{Z} + 1}{\bar{Z}} f^{1} = \frac{\partial f^{0}}{\partial z} + \frac{\tilde{E}_{z}}{v} \frac{\partial f^{0}}{\partial v}$$

$$\frac{\partial f^{1}}{\partial v} + \frac{1}{v} (3 - \bar{Z}) f^{1} = \frac{\bar{Z}}{v} \left(\frac{1}{\rho} \frac{\partial \rho}{\partial z} + \left(\frac{v^{2}}{2v_{th}^{2}} - \frac{3}{2} \right) \frac{1}{T} \frac{\partial T}{\partial z} - \frac{\tilde{E}_{z}}{v_{th}^{2}} \right) f(19)$$

3.3. The Fokker-Planck diffusive electron transport

$$v_{2th} = \sqrt{\frac{2k_BT}{m_e}} = 1/j,$$

$$A = -\frac{m_e^2 v_{2th}^2 \tilde{\mathbf{E}}}{2\pi e^4 n_e \ln \Lambda} = -\frac{mE}{2\pi j^2 e^3 n_e \ln \Lambda},$$

$$B = \frac{m_e^2 v_{2th}^4 |\nabla T|}{2\pi e^4 n_e \ln \Lambda T} = \frac{2k_B^2 T |\nabla T|}{\pi e^4 n_e \ln \Lambda},$$

$$\frac{A}{B} = -\frac{|\tilde{\mathbf{E}}|T}{v_{2th}^2 |\nabla T|},$$

$$\tilde{\mathbf{E}} = -\frac{3}{2} \frac{v_{2th}^2}{2} \frac{\gamma_T}{\gamma_E} \frac{\nabla T}{T},$$

From Eq. (24) CSR, we can write the form of f_1 including both ∇T and $\tilde{\boldsymbol{E}}$ effects as

$$f_1(v,\theta) = \cos(\theta) \frac{B}{\overline{Z}} \left(d_T(v/v_{2th}) + \frac{A}{B} d_E(v/v_{2th}) \right) f_M(v),$$

where in the case of vanishing current one gets

$$\frac{A}{B} = \frac{3}{2} \frac{\gamma_T}{2\gamma_E},$$

60 i.e.

$$f_1(v,\theta) = \cos(\theta) \frac{m_e^2}{4\pi e^4 \ln \Lambda} \frac{v_{2th}^4}{\bar{Z}} \left(2d_T(v/v_{2th}) + \frac{3}{2} \frac{\gamma_T}{\gamma_E} d_E(v/v_{2th}) \right) \frac{f_M(v)}{n_e} \frac{\nabla T}{T}, \tag{20}$$

where $d_T(x) = \bar{Z}D_T(x)/B$ and $d_E(x) = \bar{Z}D_E(x)/A$ are represented by numerical values in TABLE I and TABLE II in [5], respectively. In the case of high \bar{Z} limit, $\gamma_T \to 1$, $\gamma_E \to 1$, $d_E(x) = x^4$, and $d_T(x) = x^4(2.5 - x^2)/2$ [5], which leads to the standard Lorentz gas model

$$f_1(v,\theta) = \cos(\theta) \frac{m_e^2}{4\pi e^4 \ln \Lambda} \frac{v^4}{\bar{Z}} \left(4 - \frac{v^2}{v_{2th}^2} \right) \frac{f_M(v)}{n_e} \frac{\nabla T}{T},$$
 (21)

[2], [3], [4]

66 3.4. Summary of BGK, AWBS, and Fokker-Planck diffusion

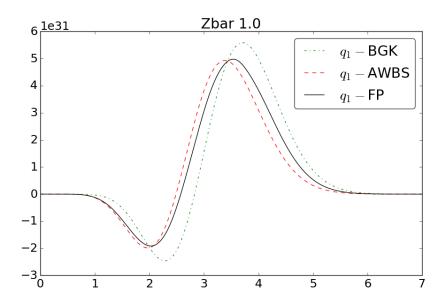


Figure 1: The flux velocity moment of the anisotropic part of the electron distribution function in low Z plasmas in diffusive regime.

	$\bar{Z}=1$	$\bar{Z}=2$	$\bar{Z}=4$	$\bar{Z} = 16$	$\bar{Z} o \infty$
$error(oldsymbol{q}_{AWBS})$	0.057	0.004	0.038	0.049	0.000

Table 1: Relative $error(q_{AWBS}) = |q_{AWBS} - q_{SH}|/q_{SH}$ of the AWBS kinetic model equation (1) showing the discrepancy (maximum around 5%) with respect to the original solution of the heat flux given by Spitzer and Harm [5].

⁶⁷ 4. Benchmarking the AWBS nonlocal transport model

58 4.1. Review of simulation codes

69 4.1.1. C7

Since in the laser heated plasmas the Knudsen number $Kn = \frac{v_{th}}{\nu_t(v_{th})L} \in$ (0,1), i.e. the collisionality in the kinetics of electrons plays always an important effect for thermal-like particles, the electron distribution function can be treated as out-of-equilibrium approximation

$$f = f_M + \delta f, \tag{22}$$

where the consequent AWBS model reads

$$v\boldsymbol{n} \cdot \nabla (f_M + \delta f) + \tilde{\boldsymbol{E}} \cdot \boldsymbol{n} \left(\frac{\partial f_M}{\partial v} + \frac{\partial \delta f}{\partial v} \right) + \frac{\tilde{\boldsymbol{E}} \cdot \boldsymbol{e}_{\theta}}{v} \frac{\partial \delta f}{\partial \theta} = v \frac{\nu_e}{2} \frac{\partial \delta f}{\partial v} + \left(\nu_{ei} + \frac{\nu_e}{2} \right) (f_0 - f_M - \delta f), \quad (23)$$

or its 1D version

$$v\mu \frac{\partial}{\partial z}(f_M + \delta f) + \tilde{\mathbf{E}}\mu \left(\frac{\partial f_M}{\partial v} + \frac{\partial \delta f}{\partial v}\right) + \frac{\tilde{E}_z(1 - \mu^2)}{v} \frac{\partial \delta f}{\partial \mu} = v\frac{\nu_e}{2} \frac{\partial \delta f}{\partial v} + \left(\nu_{ei} + \frac{\nu_e}{2}\right)(f_0 - f_M - \delta f), \quad (24)$$

where $\tilde{\boldsymbol{E}} \cdot \boldsymbol{e}_{\theta} = \tilde{E}_z \sin(\theta)$ and $\frac{\partial}{\partial \theta} = \sin(\theta) \frac{\partial}{\partial \mu}$, $\mu = \cos(\theta)$.

75 4.1.2. ALADIN

76 4.1.3. IMPACT

77 4.1.4. CALDER

78 4.2. Simulation results

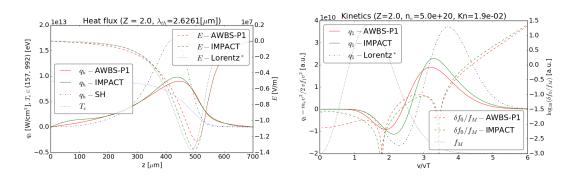


Figure 2: Snapshot 12 ps. Left: correct steady solution. Right: correct comparison to kinetic profiles at point 437 μm by IMPACT.

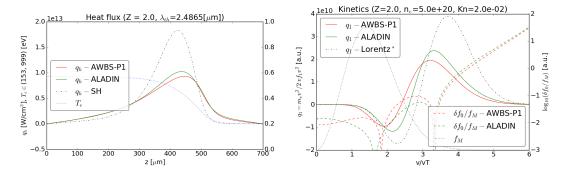


Figure 3: Snapshot 12 ps. Left: correct steady solution. Right: correct comparison to kinetic profiles at point 442 μm by ALADIN.

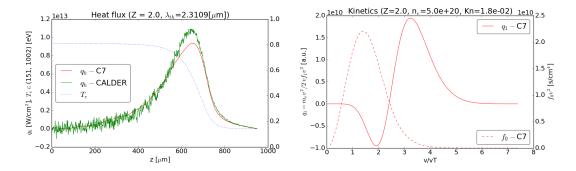


Figure 4: Snapshot 11 ps. Left: correct steady solution. Right: Kinetic profiles at point of maximum flux by C7. Kinetics profiles by CALDER to be added.

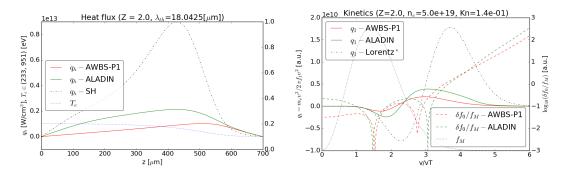


Figure 5: Snapshot 12 ps. Left: correct steady solution. Right: correct comparison to kinetic profiles at point 480 μm by ALADIN.

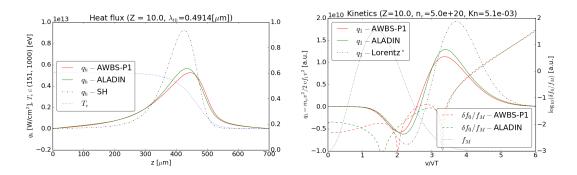


Figure 6: Snapshot 12 ps. Left: correct steady solution. Right: correct comparison to kinetic profiles at point 442 μ m by ALADIN.

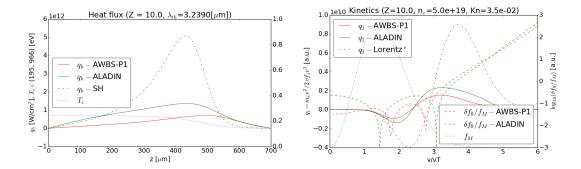


Figure 7: Snapshot 12 ps. Left: correct steady solution. Right: correct comparison to kinetic profiles at point 480 μm by ALADIN.

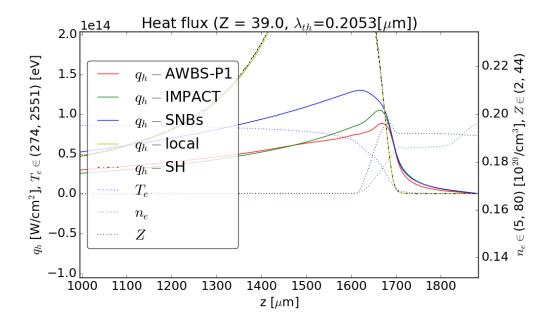


Figure 8:

⁷⁹ 5. Conclusions

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