# Boundary Conditions for the Polyatomic Gases

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Workshop on Moment Methods in Kinetic Theory II , 2014

# R19 set of equations

The regularized 19 (R19) set of equations consists of 19 PDEs for optimized moments

$$\left\{\rho, v_i, \theta, \Delta\theta, \sigma_{ij}, q_i, \Delta q_i, B^+, B^-\right\} \ ,$$

And 3 constitute equations for $B_{ij}^+$, $B_{ij}^-$ and $u_{ijk}^{0,0}$.

R19 is the polyatomic counterpart of the monatomic's R13 equations.

# Grad's 36 phase density

The generalized Grad's 36 phase density for polyatomic molecules is

$$f_{|36} = f_{int}\Big(\lambda^{0,0} + \lambda_i^{0,0} C_i + \lambda^{1,0} C^2 + \lambda^{0,0}_{<ij>} C_{<i} C_{j>} + \lambda^{0,1} e_{int}$$
$$+\lambda_i^{1,0} C_i C^2 + \lambda_i^{0,1} C_i e_{int} + \lambda^{1,0}_{<ij>} C^2 C_{<i} C_{j>} + \lambda^{2,0} C^4$$
$$+\lambda^{0,0}_{<ijk>} C_{<i} C_j C_{k>} + \lambda^{0,1}_{<ij>} C_{<i} C_{j>} e_{int} + \lambda^{1,1} C^2 e_{int}\Big) \ ,$$

This should reproduce the set of 36 raw moments

$$\{\rho, \rho\theta_{tr}, \rho\theta_{int}, \sigma_{ij}, q_{i,tr}, q_{i,int}, u^{1,0}_{ij}, u^{2,0}, u^{0,0}_{ijk}, u^{0,1}_{ij}, u^{1,1}\} \ ,$$

Therefore,

$$\lambda^{0,0} = \tfrac{4u^{1,1}+u^{2,0}}{8\rho\theta^2} + \tfrac{5}{8} - \tfrac{3(2+\delta)\theta_{tr}}{4\theta}, \quad \lambda^{0,1} = -\tfrac{u^{1,1}}{\delta\rho\theta^3} + \tfrac{15}{2\delta\theta} - \tfrac{3(5-\delta)\theta_{tr}}{2\delta\theta^2} \quad \text{and} \ \ldots$$

# Wall boundary condition

The wall boundary condition $\tilde{f}\,(c)$ is

$$\begin{cases} \chi\left[\left(1-\zeta\right)f_{tr,w}+\zeta f_{int,w}\right]+\left(1-\chi\right)f^{*}_{|36} & \mathbf{n}.\left(\mathbf{c}-\mathbf{v}_{w}\right)\succ 0\ , \\ f_{|36} & \mathbf{n}.\left(\mathbf{c}-\mathbf{v}_{w}\right)\prec 0\ . \end{cases}$$

Two equilibrium distribution functions

$$f_{tr}=\frac{\rho_{I,w}}{m}\left(\frac{1}{2\pi\theta_{w}}\right)^{\frac{3}{2}}\exp\left[-\frac{1}{2\theta_{w}}C^{2}\right]\ ,$$

$$f_{int}=\frac{\rho_{w}}{m}\frac{1}{(2\pi)^{\frac{3}{2}}\theta_{w}^{(\delta+3)/2}}\frac{1}{\Gamma\left(1+\frac{\delta}{2}\right)}\exp\left[-\frac{1}{\theta_{w}}\left(\frac{C^{2}}{2}+e_{int}\right)\right]\ .$$

# Boundary conditions

The macroscopic boundary conditions are obtained by multiplying the wall distribution function $\left(\tilde{f}\right)$ by

$$\left\{C_y,\ C_x C_y,\ C_y\left(\frac{C^2}{2}+I^{2/\delta}\right),\ C_y\left(\frac{C^2}{2}-\frac{5\,\mathrm{Pr}_{q_{int}}}{\delta\,\mathrm{Pr}_{q_{tr}}}I^{2/\delta}\right)\right.$$

$$\left.,\ C_x C_y\left(2C^2+\left(1-\frac{14}{\delta}\right)I^{2/\delta}-\frac{14+\delta}{2}\theta\right),\ C_y C_y C_y,\ C_x C_x C_y\right\}\ .$$

- Be odd in the normal component of the particle velocity.
- Fluxes should be prescribed not the variables.

# Boundary conditions

stress tensor

$$\sigma_{xy} = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi}}\left[\Upsilon V_s + \frac{5\,\mathrm{Pr}_{q_{int}}\,q_x + \delta\,\mathrm{Pr}_{q_{tr}}\,\Delta q_x}{5\left(5\,\mathrm{Pr}_{q_{int}} + \delta\,\mathrm{Pr}_{q_{tr}}\right)\sqrt{\theta}} + \frac{u^{0,0}_{xyy}}{2\sqrt{\theta}}\right] ,$$

heat flux,

$$q_y = -\frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{(56-\delta(1-\zeta))}{312}B^- + (3+\delta)\,\frac{(140+\delta(32+\delta)+(14-\delta)\delta\zeta)}{4(14+\delta)(42+25\delta)}B^-_{yy}\right.$$
$$+\frac{[(1-\zeta)\delta-4]}{312}B^+ + \frac{\delta(4-\delta(1-\zeta))}{4(42+25\delta)}B^+_{yy} - \frac{(2+\delta(1-\zeta))}{4}\theta\left(\rho\Delta\theta - \sigma_{yy}\right) + \frac{\delta(1-\zeta)}{2}\rho\theta^2$$
$$\left.+\frac{\Upsilon}{2}\sqrt{\theta}\left[(4+\delta\zeta)(\theta-\theta_w) - (1-\zeta)(\delta\theta + 3\Delta\theta) - V_s^2\right]\right]$$

where, $\Upsilon = \rho_w\sqrt{\theta_w} =$

$$-\frac{(14-\delta)(3+\delta)}{2(14+\delta)(42+25\delta)\theta^{\frac{3}{2}}}B^-_{yy} + \frac{B^+-B^-}{156\theta^{\frac{3}{2}}} - \frac{\delta B^+_{yy}}{2(42+25\delta)\theta^{\frac{3}{2}}} + \frac{\sigma_{yy}}{2\sqrt{\theta}} + \frac{\rho(2\theta-\Delta\theta)}{2\sqrt{\theta}}.$$

# Boundary conditions

## Heat flux difference

$$\Delta q_y = \frac{\chi}{(2-\chi)}\sqrt{\frac{2}{\pi\theta}}\left[\frac{15\,\Pr_{q_{int}}\Upsilon(1-\zeta)}{2\delta\,\Pr_{q_{tr}}(14+\delta)}\sqrt{\theta}\Delta\theta - \frac{5(6+\delta)\Pr_{q_{int}} - 6\delta\Pr_{q_{tr}}}{4\Pr_{q_{tr}}(42+25\delta)}B^{+}_{yy}\right.$$
$$+[3+\delta]\frac{5(42+25\delta)\Pr_{q_{int}} - 6(14-\delta)\Pr_{q_{tr}}}{4\Pr_{q_{tr}}(14+\delta)(42+25\delta)}B^{-}_{yy} - \frac{5\Pr_{q_{int}} - 4\Pr_{q_{tr}}}{2\Pr_{q_{tr}}(14+\delta)}\rho\theta^2$$
$$+\frac{5(40-\delta)\Pr_{q_{int}} - 125\delta\Pr_{q_{tr}}}{312\delta\Pr_{q_{tr}}}B^{-} + \frac{5(12+\delta)\Pr_{q_{int}} + 125\delta\Pr_{q_{tr}}}{312\delta\Pr_{q_{tr}}}B^{+}$$
$$-\frac{5(6-\delta)\Pr_{q_{int}} + 12\delta\Pr_{q_{tr}}}{4\delta\Pr_{q_{tr}}(14+\delta)}\rho\theta\Delta\theta - \frac{5\Pr_{q_{int}} - 6\Pr_{q_{tr}}}{4\Pr_{q_{tr}}(14+\delta)}\theta\sigma_{yy}$$
$$-\frac{\Upsilon}{2\Pr_{q_{tr}}(14+\delta)}\sqrt{\theta}\left[\Pr_{q_{tr}}V_s^2 - (5\Pr_{q_{int}} - 4\Pr_{q_{tr}})\,\theta\right.$$
$$\left.\left.(5\Pr_{q_{int}}\zeta - 4\Pr_{q_{tr}})(\theta - \theta_W)\right]\right]$$

Also, BCs for $B^{-}_{xy}$, $u^{0,0}_{yyy}$ and $u^{0,0}_{xxy}$.

Thanks for listening !

More info: B. Rahimi and H. Struchtrup: Capturing non-equilibrium phenomena in rarefied polyatomic gases: A high-order macroscopic model, Phys. Fluids 26, 052001 (2014).