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MATHEMATICAL MODELLING OF STEAM AND FLUE GAS FLOW IN A HEAT EXCHANGER OF A STEAM BOILER

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Abstract. We describe a transformation of the Euler equations from the conservative form to the variables of pressure, temperature and mass flow, which are preferred in the applications of the system control. This model is used to describe steam and flue gas flow in two pipes coupled by a wall with finite thickness. Then, we deal with the numerical solution of the system and suggest a variant of a finite-volume scheme which is cell-centered in pressure and temperature and vertex-centered in mass flow rate. A note on a model of the wall and an injection cooler is also included. Finally, we present a comparison with a theoretically computed temperature profile for a stationary state.

Key words. Euler equations, heat transfer, stiff systems

AMS subject classifications. 35L65, 76M12, 80A20

1. Introduction. This article is a result of development of a boiler superheating subsystem using MATLAB/Simulink environment. Main goal of our research is preparing of a modular block set which can be used for efficient modeling of a steam boiler. A full system of Euler equations is used for simulation of complete dynamics of the steam flow, not only the temperature profiles as in [4]. Another reason for using the complete Euler equations is the behavior of numerical solvers integrated in MATLAB, which exhibit tendency to fail when solving the equations of a more complex model including direct feed-through (i.e. an input affects an output directly). An example of a setup, where such problems have been observed are two chained heat exchangers modelled using equations for pressure and temperature only, and using explicitly computed mass flow [9].

The approach based on complete Euler equations does not exhibit such pathological behavior, but imposes additional demands on the used numerical method, where number of the evolution equations is significantly higher.

2. Euler equations in conservative variables. Recall that the system of Euler equations for one-dimensional flow through a pipe with constant cross-section in conservative variables reads as

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x}q = 0, \tag{2.1}$$

$$\frac{\partial}{\partial t}q + \frac{\partial}{\partial x}\left(p + \frac{q^2}{\rho}\right) = -\frac{1}{2}\zeta\frac{|q|\,q}{\rho}, \tag{2.2}$$

$$\frac{\partial}{\partial t}E + \frac{\partial}{\partial x}\left((p+E)\frac{q}{\rho}\right) = Q, \tag{2.3}$$

with ρ being density of the media, p pressure, q mass flux E energy per unit volume. This system has to be completed by the equation of state $p = p(\rho, E, q)$. The ad-

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ditional right hand side term $-\frac{1}{2}\zeta\frac{q^2}{\rho}$ describes a pressure drop due to the turbulent friction (see, e.g. [1]). The term Q in the equation of energy is volumetric heat influx.

We convert the of Euler equation in conservative variables into real variables of pressure, temperature and mass flux. Assuming that density is function of pressure and temperature only ($\rho = \rho(p, T)$), we obtain the equation of continuity as follows

$$\frac{\partial\rho}{\partial p}\frac{\partial p}{\partial t} + \frac{\partial\rho}{\partial T}\frac{\partial T}{\partial t} = -\frac{\partial q}{\partial x}. \tag{2.4}$$

Consider basic thermodynamical relations for enthalpy

$$H = U + pV, \tag{2.5}$$

where U means specific internal energy and V volume, and for internal energy U

$$E = U + \frac{1}{2}\rho V v^2, \tag{2.6}$$

where v is the velocity, and the fact that $V = 1$, we get

$$E = H + \frac{1}{2}\rho v^2 - p. \tag{2.7}$$

We substitute for E in the equation of energy:

$$\frac{\partial}{\partial t}\left(H + \frac{1}{2}\rho v^2 - p\right) + \frac{\partial}{\partial x}\left(pv + v\left(H + \frac{1}{2}\rho v^2 - p\right)\right) = Q. \tag{2.8}$$

Then, we use the relations

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho v^2\right) = \frac{1}{2}v^2\frac{\partial}{\partial t}\rho + \rho v\frac{\partial}{\partial t}v, \tag{2.9}$$

$$\frac{\partial}{\partial x}\left(\frac{1}{2}\rho v^3\right) = \frac{1}{2}v^2\frac{\partial}{\partial x}(\rho v) + \rho v^2\frac{\partial}{\partial x}v. \tag{2.10}$$

and the equation of continuity. By differentiation, we obtain

$$\frac{\partial H}{\partial p}\frac{\partial p}{\partial t} + \frac{\partial H}{\partial T}\frac{\partial T}{\partial t} - \frac{\partial p}{\partial t} + \rho v\frac{\partial v}{\partial t} + \frac{\partial}{\partial x}(vH) + \rho v^2\frac{\partial v}{\partial x} = Q. \tag{2.11}$$

In the equation of momentum conservation,

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(p + \rho v^2) = -\frac{1}{2}\zeta\rho\,|v|\,v, \tag{2.12}$$

we use the equation of continuity and multiply by v. Consequently

$$\rho v\frac{\partial v}{\partial t} + v\frac{\partial p}{\partial x} + \rho v^2\frac{\partial v}{\partial x} = -\frac{1}{2}\zeta\rho\,|v|^3\,. \tag{2.13}$$

Subtracting (2.13) from (2.11), we get

$$\frac{\partial H}{\partial p}\frac{\partial p}{\partial t} + \frac{\partial H}{\partial T}\frac{\partial T}{\partial t} - \frac{\partial p}{\partial t} = \frac{q}{\rho}\frac{\partial p}{\partial x} + \frac{1}{2}\zeta\frac{1}{\rho^2}\,|q|^3 - \frac{\partial}{\partial x}(vH) + Q. \tag{2.14}$$

Then, it is possible to compute the derivatives of $\frac{\partial p}{\partial t}$ a $\frac{\partial T}{\partial t}$ from the equations (2.4) and (2.14):

$$A_1 \frac{\partial p}{\partial t} = -\frac{\partial H}{\partial T}\frac{\partial q}{\partial x} - \frac{\partial \rho}{\partial T} A_2, \tag{2.15}$$

$$A_1 \frac{\partial T}{\partial t} = -\left(1 - \frac{\partial H}{\partial p}\right)\frac{\partial q}{\partial x} + \frac{\partial \rho}{\partial p} A_2, \tag{2.16}$$

where

$$A_1 = \frac{\partial \rho}{\partial p}\frac{\partial H}{\partial T} + \left(1 - \frac{\partial H}{\partial p}\right)\frac{\partial \rho}{\partial T}, \tag{2.17}$$

$$A_2 = \frac{q}{\rho}\frac{\partial p}{\partial x} + \frac{1}{2}\zeta\frac{|q|^3}{\rho^2} - \frac{\partial}{\partial x}\left(\frac{q}{\rho}H\right) + Q. \tag{2.18}$$

These two equations together with equation of momentum (2.2) and state equations

$$\left[\rho, \hat{H}, \frac{\partial \rho}{\partial p}, \frac{\partial \rho}{\partial T}, \frac{\partial \hat{H}}{\partial p}, \frac{\partial \hat{H}}{\partial T}\right] = f(p, T), \tag{2.19}$$

where $\hat{H}$ is the specific enthalpy, form the evolution equations in state variables (p,T,q). Values of $\frac{\partial H}{\partial p}$ and $\frac{\partial H}{\partial T}$ can be easily computed using the Leibniz rule

$$\frac{\partial H}{\partial p} = \frac{\partial \rho}{\partial p}\hat{H} + \rho\frac{\partial \hat{H}}{\partial p}, \tag{2.20}$$

$$\frac{\partial H}{\partial T} = \frac{\partial \rho}{\partial T}\hat{H} + \rho\frac{\partial \hat{H}}{\partial T}. \tag{2.21}$$

To complete the system of equations, we have to provide the equations of state. In the case of steam, the equations we are using are based on the Steam Properties Tables [11]. We currently use a polynomial approximation of the table values, which also allows computation of partial derivatives.

Regarding the choice of the boundary conditions, as we consider the sub-sonic flow, it is reasonable to impose two Dirichlet-type boundary conditions at the inlet and one at the outlet. We decided to prescribe the steam pressure and temperature at the inlet, and mass flux at the outlet.

For flue gas we use a state equation of an ideal nitrogen, because it constitutes the largest portion of it, determining the behavior of the mixture. Thus, for enthalpy we consider the relation

$$\hat{H} = c_p T \tag{2.22}$$

and for density it holds that

$$\rho = \frac{pM}{RT}, \tag{2.23}$$

where

$$M = 0.02801\,\mathrm{kg\,mol^{-1}}$$

is the molar mass of nitrogen,

$$c_p = 1037.0\,\mathrm{J\,kg^{-1}\,K}$$

specific thermal capacity for constant pressure and

$$R = 8.3144\,\mathrm{J\,mol^{-1}\,K^{-1}}$$

molar gas constant.

3. Numerical solution of the steam/flue gas flow. We discretize (2.15) and (2.16) by replacing spatial derivatives with differences, and we obtain the following set of equations for $i = \{1, \ldots, n\}$, where n is the number of cells. The values of p_j, T_j, q_j for $j = \{0, n+1\}$ are either determined using corresponding boundary condition, or obtained by linear extrapolation from the domain.

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = \frac{1}{A_1}\left(-\left(\left.\frac{\partial\rho}{\partial T}\right|_i \hat{H}_i + \rho_i \left.\frac{\hat{H}}{\partial T}\right|_i\right)\Delta_x q_i - \left.\frac{\partial\rho}{\partial T}\right|_i A_2\right), \tag{3.1}$$

$$\frac{\mathrm{d}T_i}{\mathrm{d}t} = \frac{1}{A_1}\left(-\left(1-\left(\left.\frac{\partial\rho}{\partial p}\right|_i \hat{H}_i + \rho_i \left.\frac{\partial\hat{H}}{\partial p}\right|_i\right)\right)\Delta_x q_i + \left.\frac{\partial\rho}{\partial p}\right|_i A_2\right), \tag{3.2}$$

$$\frac{\mathrm{d}q_{i-1,i}}{\mathrm{d}t} = \frac{1}{\Delta x_i}\left(P_{i-1} - P_i + q_{i,i-1}^2\left(\frac{1}{\rho_{i-1}} - \frac{1}{\rho_i}\right)\right) - \frac{1}{4}\zeta q_{i-1,i}\left(\frac{1}{\rho_{i-1}} + \frac{1}{\rho_i}\right) \tag{3.3}$$

where

$$A_1 = \left.\frac{\partial\rho}{\partial p}\right|_i\left(\left.\frac{\partial\rho}{\partial T}\right|_i \hat{H}_i + \rho_i \left.\frac{\partial\hat{H}}{\partial T}\right|_i\right) + \left(1-\left(\left.\frac{\partial\rho}{\partial p}\right|_i \hat{H}_i + \rho_i \left.\frac{\partial\hat{H}}{\partial p}\right|_i\right)\right)\left.\frac{\partial\rho}{\partial T}\right|_i, \tag{3.4}$$

$$A_2 = \frac{q_i}{\rho_i}\Delta_x p_i + \frac{1}{2}\zeta\frac{q_i^3}{\rho_i^2} + \Delta_x(q_i\hat{H}_i) - Q, \tag{3.5}$$

$$\Delta_x\{\cdot\} = \frac{\{\cdot\}_R - \{\cdot\}_L}{\Delta x} \tag{3.6}$$

and $\{\cdot\}_L$, $\{\cdot\}_R$ denote values at the left and right volume interface.

Value of mass flow q in the cell is approximated by a simple average of the values at the left and right interfaces. The values of H and p at the cell boundaries are approximated by a piece-wise linear interpolation using the minmod slope limiter and upwinding (see [3], [13]). Since in our case we suppose uni-directional flow, the formulas thus can be reduced to backward differencing.

A deeper theoretical analysis of the numerical approximation is beyond the scope of this article. However, after performing several numerical experiments involving both studying reactions on the jumps in the input quantities and fitting the model to reflect the behavior of a real world setup, this particular choice of numerical method seems to behave well. For our purpose, it is important that it gives reasonable results for very sparse meshes (about 10 points for a 60 meters long exchanger pipe). This allows for a real-time simulation of the system, which is crucial for the system control applications.

For the choice of a suitable ODE solver, it is important to take into account, that the boiler itself has properties of a stiff system, because the processes related to the steam flow are faster than the processes related to the heat transfer in several orders of magnitude (see [14]).

4. Pipe wall model and the thermal transfer. Temperature of the exchanger pipe wall is given by the heat equation

$$S_3\left(\rho_3 c_3 \frac{\partial T^{(3)}}{\partial t} - \frac{\partial}{\partial x}\left(\lambda \frac{\partial T^{(3)}}{\partial x}\right)\right) = -Q, \tag{4.1}$$

with S_3 being the wall cross-section, c_3 specific heat capacity, $T^{(3)}$ wall temperature, λ thermal conductivity and Q linear heat transfer density out of the wall.

For linear heat transfer density, we consider following relations:

$$Q^{(1)} = o_1\alpha_1(T^{(3)} - T^{(1)}), \tag{4.2}$$

$$Q^{(2)} = o_2\alpha_2(T^{(3)} - T^{(2)}), \tag{4.3}$$

$$Q = Q^{(1)} + Q^{(2)}, \tag{4.4}$$

where $o_{1,2}$ is an effective pipe perimeter and $T^{(1)}$, $T^{(2)}$ and $T^{(3)}$ are temperatures of the steam, flue gas and pipe wall, respectively.

Formulas for the transmission coefficient α are presented in [5] and [6]. An empirical relation for an aligned tube bundle is

$$\alpha = \frac{Nu\lambda_f}{D_f},\ Nu = 0.202K_1Re^{0.64}Pr^{0.4}, Re = \frac{u_f D_f}{\nu}, Pr = \frac{\lambda}{\rho c \nu} \tag{4.5}$$

where ν is the kinematic viscosity, D_f outer tube diameter, u_f fluid velocity and K_1 fitting constant. Re, Pr and Nu are Reynolds number, Prandtl number and Nusselt number, respectively.

The heat equation describing the wall can be easily solved using method of lines. This method has also an advantage that it can be incorporated into MATLAB/Simulink framework [14]. The heat transfer equation is discretized in space, yielding the following set of ordinary differential equations.

$$\frac{\mathrm{d}T_i^{(3)}}{\mathrm{d}t} = \frac{1}{\rho c}\left(\lambda \frac{T_{i-1}^{(3)} - 2T_i^{(3)} + T_{i+1}^{(3)}}{\Delta x^2} - \frac{Q_i}{S}\right). \tag{4.6}$$

The wall model can be further simplified, because the thermal transfer coefficient λ and the wall cross-section are fairly small and thermal transfer along the wall can be neglected. In that case, the (discretized) wall model reduces to

$$\frac{\mathrm{d}T_i}{\mathrm{d}t} = -\frac{1}{\rho c}\frac{Q_i}{S}. \tag{4.7}$$

5. Model of an injection cooler. The temperatures in the steam pipes are regulated using the injection coolers. These devices are basically small chambers with a jet where the cooling water is injected to lower the overall steam temperature. The injection-cooler model we propose follows the idea of [5]. We neglect the pressure drop in the cooler element so that model reflects only dynamics of output-temperature change. Mass balance in the cooler implies (in the following, all the mass fluxes are specified in $\mathrm{kg\,s^{-1}}$, rather than $\mathrm{kg\,s^{-1}\,m^{-2}}$). V is an internal volume of the cooler, q_{in} q_{out}, and q_{w} are the input, output and cooling water fluxes. Quantities $\hat{H}_{\mathrm{in}}$, $\hat{H}_{\mathrm{w}}$ and $\hat{H}$ are enthalpy of the steam at the inlet, enthalpy of the cooling water and enthalpy of the steam in the cooler.

$$V\frac{d\rho}{\mathrm{d}t} = q_{\mathrm{in}} + q_{\mathrm{w}} - q_{\mathrm{out}} \tag{5.1}$$

and from the energy balance, we have

$$V\frac{\mathrm{d}}{\mathrm{d}t}(\rho\hat{H}) = q_{\mathrm{in}}\hat{H}_{\mathrm{in}} + q_{\mathrm{w}}\hat{H}_{\mathrm{w}} - q_{\mathrm{out}}\hat{H}. \tag{5.2}$$

Multiplying (5.1) by $\hat{H}$ and subtracting it from (5.2), we obtain

$$V\rho\frac{\mathrm{d}\hat{H}}{\mathrm{d}t} = q_{\mathrm{in}}\hat{H}_{\mathrm{in}} + q_{\mathrm{w}}\hat{H}_{\mathrm{w}} - (q_{\mathrm{in}} + q_{\mathrm{w}})\,\hat{H}. \tag{5.3}$$

For the steady state, enthalpy of the mixture is

$$\hat{H} = \frac{q_{\mathrm{in}}\hat{H}_{\mathrm{in}} + q_{\mathrm{w}}\hat{H}_{\mathrm{w}}}{q_{\mathrm{in}} + q_{\mathrm{w}}}. \tag{5.4}$$

Using the state equations $\rho = \rho(p,T)$ and $\hat{H} = \hat{H}(p,T)$, we can rewrite (5.1) and (5.3) to the following form:

$$V\begin{bmatrix} \frac{\partial\rho}{\partial p} & \frac{\partial\rho}{\partial T} \\ \rho\frac{\partial\hat{H}}{\partial p} & \rho\frac{\partial\hat{H}}{\partial T} \end{bmatrix}\begin{bmatrix} \frac{\partial p}{\partial t} \\ \frac{\partial T}{\partial t} \end{bmatrix} = \begin{bmatrix} q_{\mathrm{in}} + q_{\mathrm{w}} - q_{\mathrm{out}} \\ q_{\mathrm{in}}\hat{H}_{\mathrm{in}} + q_{\mathrm{w}}\hat{H}_{\mathrm{w}} - (q_{\mathrm{in}} + q_{\mathrm{w}})\hat{H} \end{bmatrix}. \tag{5.5}$$

As the hydraulic resistance of the cooler can be omitted we may assume that $p = p_{\mathrm{in}}$. When we also neglect the terms containing $\frac{\mathrm{d}p}{\mathrm{d}t}$, the system (5.5) can be rewritten to the form

$$\begin{bmatrix} V\frac{\partial\rho}{\partial T} & -1 \\ V\rho\frac{\partial\hat{H}}{\partial T} & \hat{H} - \hat{H}_{\mathrm{in}} \end{bmatrix}\begin{bmatrix} \frac{\mathrm{d}T}{\mathrm{d}t} \\ q_{\mathrm{in}} \end{bmatrix} = \begin{bmatrix} q_{\mathrm{w}} - q_{\mathrm{out}} \\ q_{\mathrm{w}}(\hat{H}_{\mathrm{w}} - \hat{H}) \end{bmatrix}. \tag{5.6}$$

From the first row we get

$$q_{\mathrm{in}} = q_{\mathrm{out}} - q_{\mathrm{w}} + V\frac{\partial\rho}{\partial T}\frac{\mathrm{d}T}{\mathrm{d}t}. \tag{5.7}$$

Substitution of (5.7) into the second equation of (5.6) gives

$$V\left((\hat{H} - \hat{H}_{\mathrm{in}})\frac{\partial\rho}{\partial T} + \rho\frac{\partial\hat{H}}{\partial T}\right)\frac{\mathrm{d}T}{\mathrm{d}t} = (\hat{H}_{\mathrm{w}} - \hat{H}_{\mathrm{in}})q_{\mathrm{w}} - (\hat{H} - \hat{H}_{\mathrm{in}})q_{\mathrm{out}}. \tag{5.8}$$

In many cases we can neglect the cooler dynamics at all and use a static model. Linearized expression for the specific enthalpy is

$$\hat{H} - \hat{H}_{\mathrm{in}} = \hat{H}(p_{\mathrm{in}},T) - \hat{H}(p_{\mathrm{in}},T_{\mathrm{in}}) = \frac{\partial\hat{H}}{\partial T}(T - T_{\mathrm{in}}). \tag{5.9}$$

With $\frac{\mathrm{d}T}{\mathrm{d}t} = 0$, (5.8) then simplifies to

$$T = T_{\mathrm{in}} - \frac{\hat{H}_{\mathrm{in}} - \hat{H}_{\mathrm{w}}}{\frac{\partial\hat{H}}{\partial T}}\frac{q_{\mathrm{w}}}{q_{\mathrm{out}}} \tag{5.10}$$

and the mass outflow is

$$q_{\mathrm{out}} = q_{\mathrm{in}} + q_{\mathrm{w}}. \tag{5.11}$$

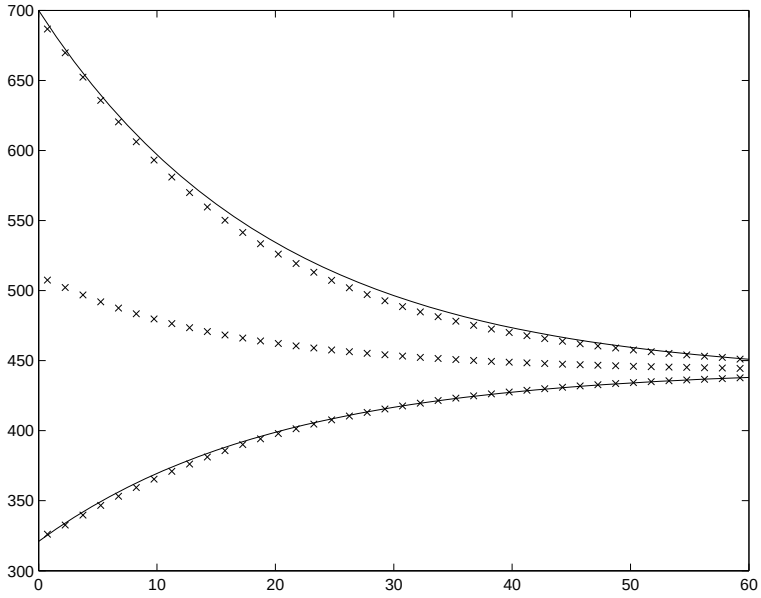

FIG. 6.1. *Stationary temperature profiles. x-axis: x-coordinate in meters, y-axis: temperature in °C.*

6. Stationary flow in heat exchangers. When we impose additional simplifying assumptions, it is possible to treat the problem of finding the stationary state by solving a system of ordinary differential equations. Using [4], we are able to find temperature profiles in parallel heat exchangers, and compare the theoretical profiles with the results obtained by our numerical simulation.

Let us denote mass fluxes in the pipes a and b by q_a and q_b. We assume that the velocity and all thermodynamical quantities except temperature T are constant. We look for a stationary solution to the transport equations

$$S_a \rho_a c_a \left(\frac{\partial T_a}{\partial t} + v_a \frac{\partial T_a}{\partial x} \right) = Q_a, \tag{6.1}$$

$$S_b \rho_b c_b \left(\frac{\partial T_b}{\partial t} + v_b \frac{\partial T_b}{\partial x} \right) = Q_b, \tag{6.2}$$

where we do not consider any heat capacity of the wall. Consequently a direct Newton-type heat exchange occurs between the two media:

$$Q_a = k(T_b - T_a), \quad Q_b = k(T_a - T_b). \tag{6.3}$$

The constant k denotes the linear heat transfer coefficient, e.g $k = \alpha \cdot o$, where α is the heat transfer coefficient and o denotes effective perimeter of the pipe. The equations (6.1), (6.2) can be solved analytically. The solution is

$$T_a(x) = \frac{T_{a1} - T_{a_2}}{1 - e^{-CL}} \left(e^{-Cx} - 1 \right) + T_{a_1}, \tag{6.4}$$

$$T_b(x) = \frac{T_{b1} - T_{b_2}}{1 - e^{-CL}} \left(e^{-Cx} - 1 \right) + T_{b_1} \tag{6.5}$$

with

$$C = k\left(\frac{1}{c_a q_a} + \frac{1}{c_b q_b}\right), \tag{6.6}$$

for $x \in [0, L]$ and T_{a_1} and T_{b_1} are the temperatures of the media at the inlets.

In the Figure 6.1 we present the typical temperature profiles for a model of a convection superheater, which was however slightly modified to allow comparison with the simplified equations above. The heat transfer coefficient is constant and is the same for both steam and flue gas and the lengths of the steam and gas pipes are identical. The crosses represent the discrete values of temperature obtained by a numerical simulation and the full lines represent the temperatures of the steam and flue gas obtained by the theoretical solution. To make the exponentials (6.4) fit in this case, the constant k has to be chosen about two times lower than the heat transfer coefficient in the numerical simulation would suggest. This can be attributed to the effect of the wall, which retains the temperature approximately in the middle.

7. Conclusion. The current version of the heat exchanger model has been tested and the full system of equations without a direct link between inputs and outputs behaves well even in the setup with more heat exchangers with injection coolers between them. For the future, we plan connecting this model with a model of phase changes in the evaporator and eventually with a combustion simulation.

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