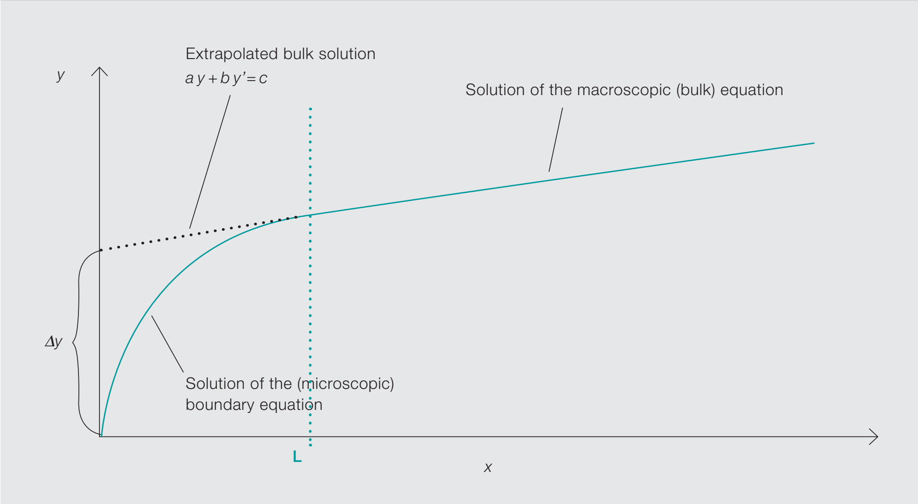
Boundaries of knowledge

Knowledge of boundary conditions is crucial for reliable simulations

KAI HENCKEN, THOMAS CHRISTEN – Partial differential equations (PDEs) are the basic language with which physicists describe many natural phenomena, such as electric and magnetic fields, acoustics, fluid flow, and heat conduction. The PDEs that describe the physics inside a spatial domain of interest – so-called bulk equations – are the key elements in numerical simulations of ABB products [1]. However, at the boundaries of many systems the variety of underlying physical processes that need to be taken into account is far richer than in the bulk. In addition, boundaries often govern the result of a simulation even though they only occupy a small part of the whole system. Hence, in obtaining meaningful numerical simulations, appropriate boundary conditions can play a decisive role. Describing these mathematically is, in general, not an easy task and requires a deep insight into the underlying physics.

1 Derivation of boundary conditions for a macroscopic equation from the underlying microscopic physics



PDEs describe the behavior of physical properties or quantities in space and time. Typical examples are the heat equation for temperature, the Laplace equation for electric potential, and the fluid dynamics equations for mass, momentum and energy flow.

The occurrence of (mathematical) spatial derivatives in these PDEs is associated with a coupling of a given point in space with its surroundings, often due to a transport phenomenon. In order to obtain well-defined, ie, unique, solutions of the PDEs, boundary conditions must be specified. This is similar to the requirement for an initial condition in order to solve for a time-dependent process – the conditions at the starting time of a simulation can be interpreted as a boundary condition for the time axis, as an analogy. The general mathematical form of specific boundary conditions mainly depends on two structural properties of the bulk equations.

Title picture
Products contain many internal boundaries, surfaces and interfaces that strongly determine their performance and which must be described in simulations by boundary conditions.

The first property is the order of the PDE, which indicates the highest spatial derivative that occurs in the bulk equation. For instance, the heat equation is of order two, as a derivative of the form $\partial^2 T/\partial x^2$ occurs. The boundary conditions will, in general, be a relation between the physical quantities and their (spatial) derivatives with an order smaller by one than the order of the PDE itself, because higher order derivatives can be eliminated with the help of the bulk PDE. For instance, in the steady-state heat equation, $\partial^2 T/\partial x^2=0$, the boundary condition might, in principle, contain arbitrary spatial derivatives, not only T itself and its derivative. But terms of the form “$\partial^2 T/\partial x^2$” or higher can be eliminated using $\partial^2 T/\partial x^2=0$.

The second property concerns how information propagates inside the bulk, ie, how a disturbance or change of a physical quantity at one point influences its value at a distance at the same or a later time.

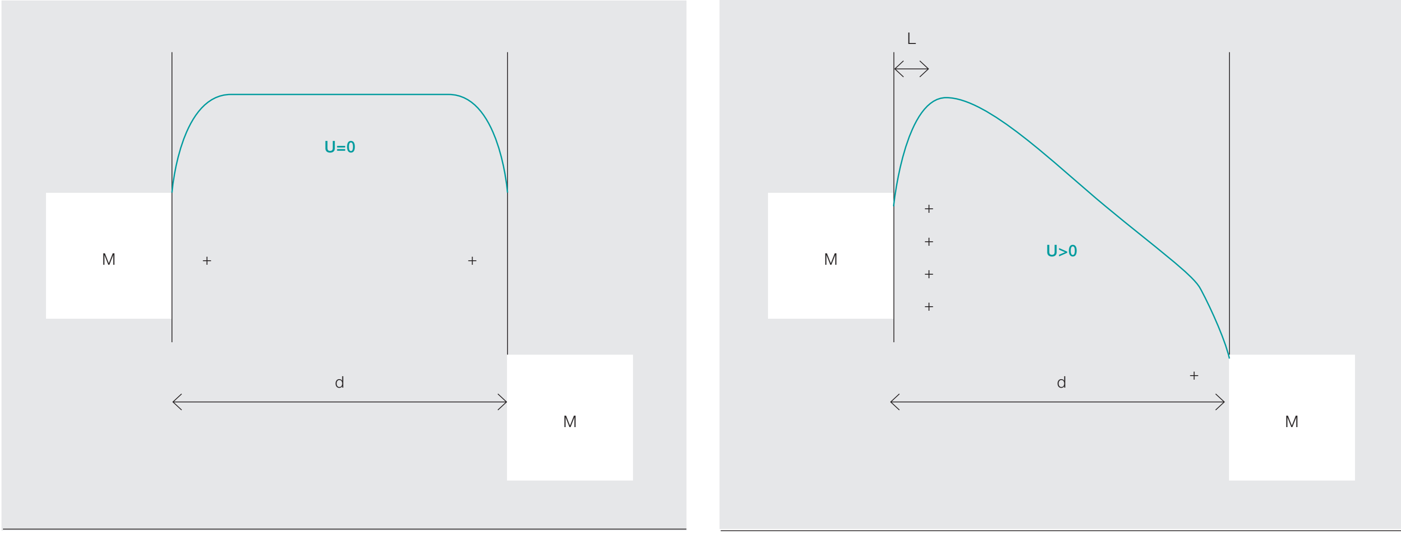
The simplest example is a PDE of order zero. Spatial derivatives and propagation are then absent and boundary conditions are superfluous. The equation is, in this case, a (distributed) system of ordinary differential equations (ODEs) rather than a PDE. A physical example of this is the electric polarization induced in a dielectric medium, which can be described by a relaxation process of the local polarization density.

For meaningful numerical simulations, bulk models have to be complemented with appropriate boundary conditions.

There are other cases where a boundary condition is unnecessary, even if spatial derivatives occur. For instance, the state of a supersonic fluid at an outlet is completely determined by the information coming from the bulk. Because the fluid flows faster than the speed of sound, which is the information velocity in this case, no information can flow backward from the boundary into the bulk. Hence, this boundary will not affect the state in the bulk.

Boundary conditions are usually necessary and are classified according to the propagation behavior of the PDEs – diffusive, instantaneous, convective or wavelike. For example, instantaneous propagation corresponds to steady-state solutions, where one implicitly assumes that the propagation and, therefore, the equilibration, in the system is much faster than the timescale considered. An example is the formation of an electric field (eg, in a vacuum), which is usually described by the instantaneous Laplace equation.

2 Ohmic contact



2a Insulator without intrinsic, but with injected, charge carriers (here positive holes) from the two attached electrode contacts. (Blue: equilibrium potential.)

2b Application of a voltage tilts the energy potential seen by the carriers, leading to a maximum near the injecting electrode.

The boundary conditions have to be formulated in a way that makes the model well-posed, ie, a physically reasonable solution exists.

Transients can in practice often be disregarded due to the fact that the electric field travels with the speed of light.

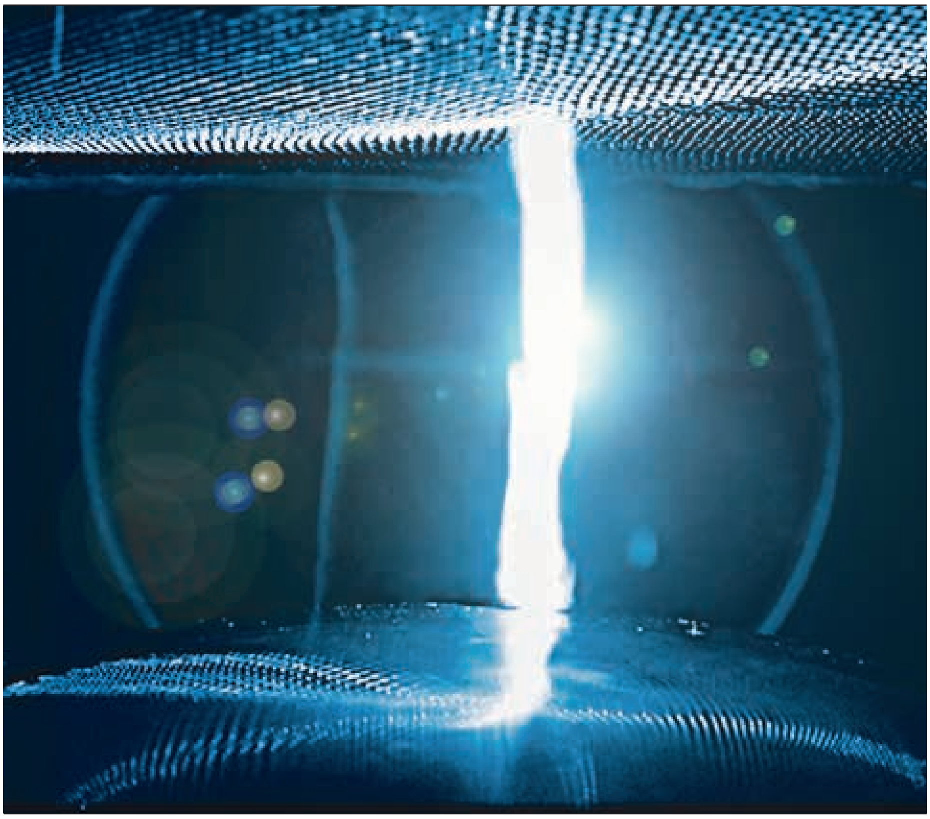
The boundary conditions have to be formulated in a way that makes the model well-posed – ie, a physically reasonable solution exists. This can impose restrictions on the number and types of conditions that are needed at each boundary.

Boundary condition physics goes beyond bulk physics

As mentioned, the bulk equations constrain and prescribe the functional form of the boundary conditions. However, the values of the coefficients or parameters occurring in them are still free and need to be determined by the underlying physics. This can be a sophisticated task, as boundary conditions need a more detailed view into the physical system than the bulk PDEs. Bulk PDEs are derived by averaging quantities, like thermal energy, over small volume elements in which these quantities are considered homogenous. At boundaries, the properties change abruptly, making consideration on a shorter, eg, microscopic, scale necessary. As a consequence, boundary condition modeling must take physics at a higher level of detail and greater variety of phenomena than the bulk equation into account.

An important example of this is represented by bulk equations for a gas under the assumption of local thermodynamic equilibrium, where the temperature is well-defined and the velocities of the particles follow the Maxwell distribution. When approaching the boundary, this velocity distribution deviates from the one in the bulk due to surface effects and thermodynamic equilibrium is no longer a given → 1. In other words, the macroscopic equations for the physical quantity $y(x, t)$ along the x-axis of → 1 are valid for distances larger than a certain microscopic length L, but not below it. The magnitude of this boundary region is assumed to be much smaller than the scale that is resolved in the numerical simulation. The extrapolation of the bulk solution to the boundary does not necessarily coincide with the microscopic solution. However, the boundary condition has to fulfill the mathematical relation set by the bulk equation.

3 An electric arc burning between two electrodes.
The arc root forms an interesting and complex boundary.



In this case it is given by a general relation of the form

$$ay+by'=c$$

The coefficients a, b and c must be obtained by enforcing a smooth transition from the microscopic to the macroscopic solution. For instance, even if the fundamental microscopic physics calls for $y=0$ at the boundary $(x=0)$, the macroscopic boundary condition may exhibit a discontinuity due to the physics in the microscopic boundary layer. An important example is a slip boundary condition for the (macroscopic) gas flow velocity in a pipe, where one assumes a finite velocity all the way to the wall, although microscopically, ie, in a very thin viscous boundary layer, it rapidly decreases to zero at the wall.

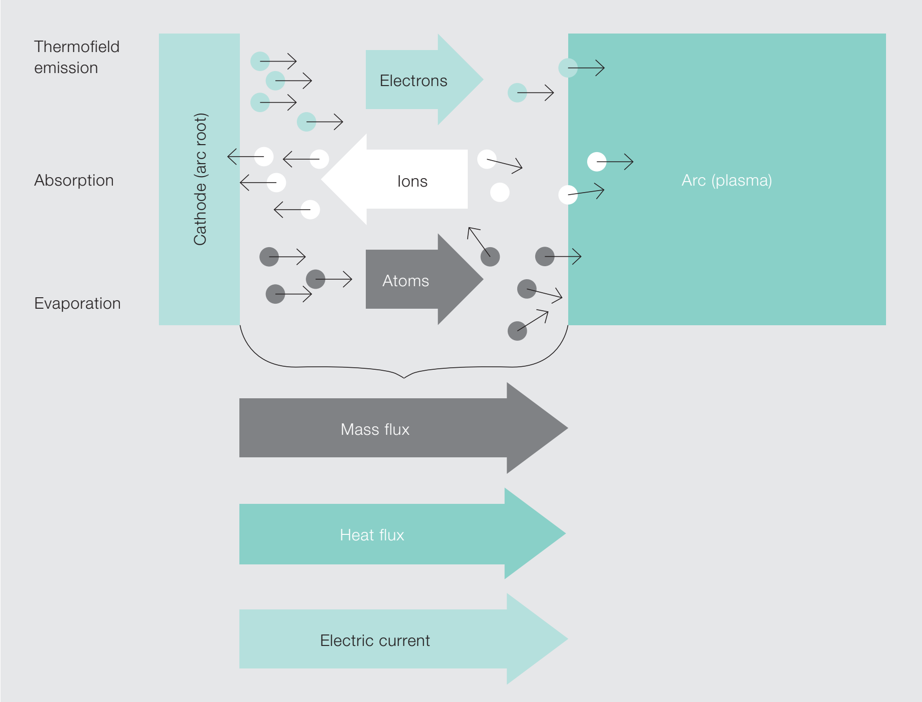
> The underlying physics that needs to be taken into account at boundaries is much richer than for bulk equations.

DC conduction in insulators

In AC cables, the 50 Hz field distribution is usually calculated by solving a Laplace equation for the electric potential in the dielectric materials, with appropriate boundary conditions on the conductive parts. The relevant material property is the dielectric permittivity and any accumulation of charges within the dielectric materials can be neglected.

Field calculations in DC insulation, however, are considerably more complex because space charges can build up inside the material. By this, sometimes very slow, process, the field distribution may change significantly over time. An illustrative example of the coupled interaction of the boundary with the bulk is the formation of a space-charge-limited current (SCLC): Consider a material that is initially bare of any charge carriers and with a metal contact on each side ➔ 2. Even without an applied voltage, charge carriers (positive holes, say, for simplicity) will diffuse from the electrodes into the insulator.

4 A number of physical phenomena occur in an arc root – only the microscopic view shows the interdependency between them.



Charge injection from electrodes can be of great relevance when designing HVDC cable and accessories.

There, they create a thin charge accumulation layer that leads to an increased, almost flat, potential distribution in the interior of the insulator. The electric field, which is essentially the negative slope of the potential, is thus practically zero everywhere between the plates, except near the contacts ➔ 2a. A high voltage applied across the electrodes induces a strong tilt of the potential that leads to a potential maximum near one of the electrodes ➔ 2b.

Typically, this distance is too small to be resolved in the macroscopic simulation and is excluded. But this maximum has important consequences. The electric field is zero at the maximum, as it is, by definition, the slope of the potential. This location is called the "virtual electrode" and electrodes that exhibit this property of vanishing field under these conditions are named "ohmic electrodes." Because the electric current – which is proportional to the product of the electric field, the charge carrier density and their mobility – remains finite, a vanishing electric field together with a nonzero current implies that the charge carrier density diverges (becomes infinite) at the virtual electrode. In reality, the density remains, of course, finite due to the action of diffusion, which was, in this simple picture, neglected. The electrode injects a large number of charge carriers, leading to such a large charge density at the contact that the electric field is suppressed. This can lead to a field enhancement at another place or after polarity reversal.

Charge injection and accumulation is of great relevance when designing HVDC insulation devices. A main consequence of it is that the electric field distribution is then not only determined by a bulk conductivity, but is also influenced by contacts and the boundary between them, which requires special measures to make HVDC insulation robust [2].

Arc roots in vacuum circuit breakers

In vacuum circuit breakers (VCBs), the interruption of currents occurs via the formation and extinction of an electric arc [3] ➔ 3. First of all, as the bulk mate-

Circuit breakers rely strongly on boundary effects – for example, metal vaporization in vacuum breakers and nozzle ablation in gas circuit breakers.

rial here is vacuum, the relevance of appropriate boundary conditions is obvious because the metal plasma in the VCB completely originates from the electrodes. Secondly, the example presents a complex multiphysics boundary problem, since a number of different physical phenomena are involved that can be treated independently in the bulk, but are connected at the lower level.

Arc roots are the areas where the arc connects to the metal electrodes. An electric layer is formed at an arc root. This non-neutral sheath leads to a voltage between the bulk of the plasma and the electrode – ie, the electrode voltage drop, similar to what is shown in ➔ 2a. This voltage drop leads to a strong electric field at the surface. This is needed to draw a large electric current from the metal to the plasma by making electrons leave the cathode or enter the anode and by making ions move to the surface ➔ 4. This ion movement and recombination is the dominant heating mechanism for the metal. The electrode surface in the arc root becomes so hot that metal evaporates. The vacuum arc is actually a metal vapor arc that feeds itself purely from the material emitted from the arc roots. The balance of the surface heating from the plasma and the cooling by metal evaporation determines the electrode temperature and, by this, the performance of the breaker.

Each of these processes is complex in itself, but, because the same particles (electrons, ions and atoms) are the carriers of different properties (mass, heat and electric current), the boundary conditions are interrelated and this has to be taken into account if a consistent simulation is to be obtained.

Another example of the relevance of boundary effects is found in arc-radiation-induced material ablation in gas circuit breakers, which is relevant for the pressure buildup needed in the switching process [1].

Further examples are to be found in sensors, oil-insulated HV equipment and so on.

Reliable simulation

For meaningful numerical simulations, bulk models have to be complemented with appropriate boundary conditions. Boundaries often have a substantial effect on the result even though they only occupy a small part of the whole system. Furthermore, the variety of underlying physical processes that need to be taken into account in boundaries is much richer than in the bulk, whose equations often follow from simplifying conservation laws.

It is wise, when validating simulation results, to scrutinize the boundary conditions used, for two reasons: First, due to their large effect, it is sometimes easy to produce the desired results by tuning boundary condition parameters. Second, the physics behind boundary conditions is often very complex and can be treacherous. Choosing a good boundary condition is not an easy task and requires a deep insight into the underlying physics, but the effort pays off by delivering much more reliable simulation results. Last but not least, an understanding of the governing boundary physics can be an important source of technical innovation.

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